Online Optimizing Control: The Link between Plant Economics and Process Control

Sebastian Engell

Process Dynamics and Operations Group
Department of Biochemical and Chemical Engineering
Technische Universität Dortmund
Dortmund, Germany

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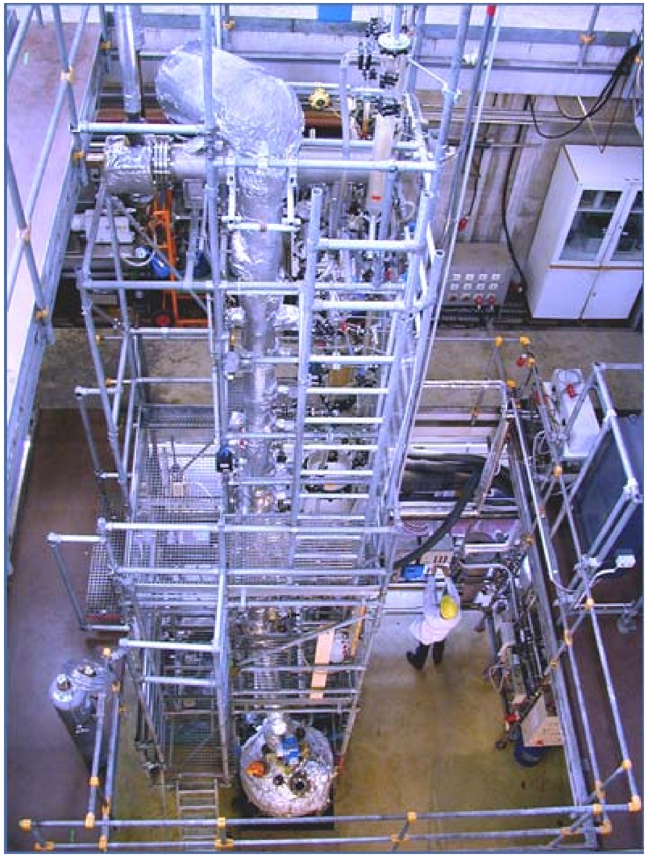
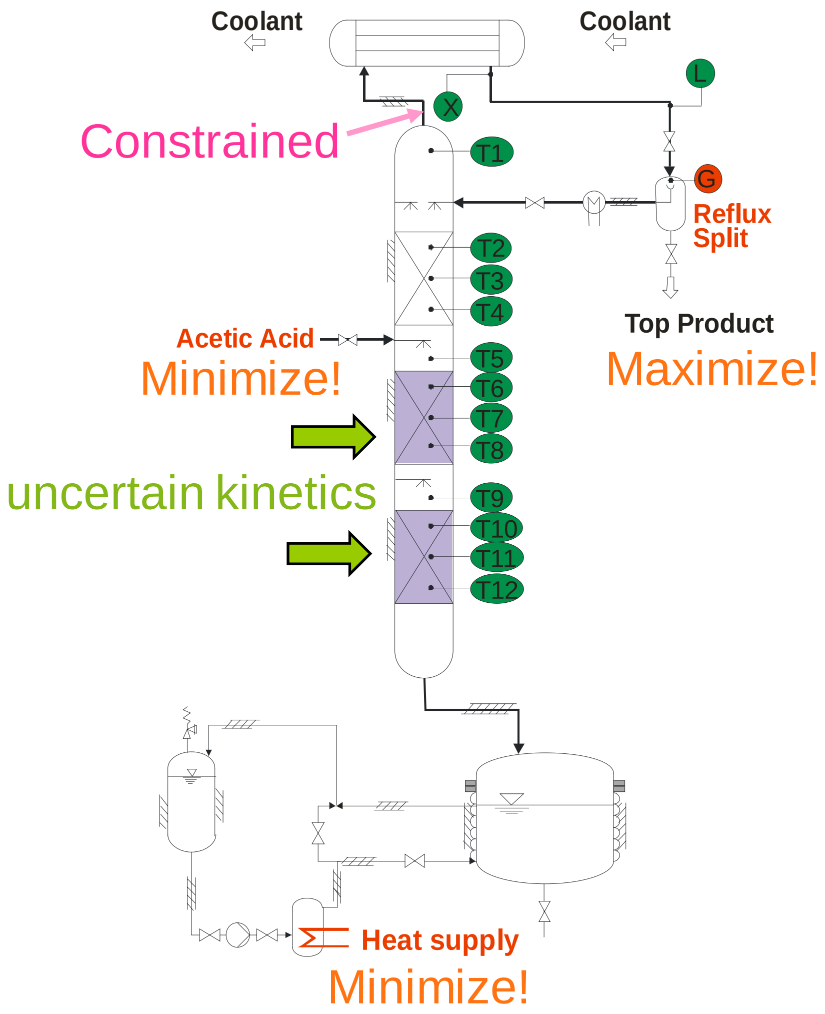
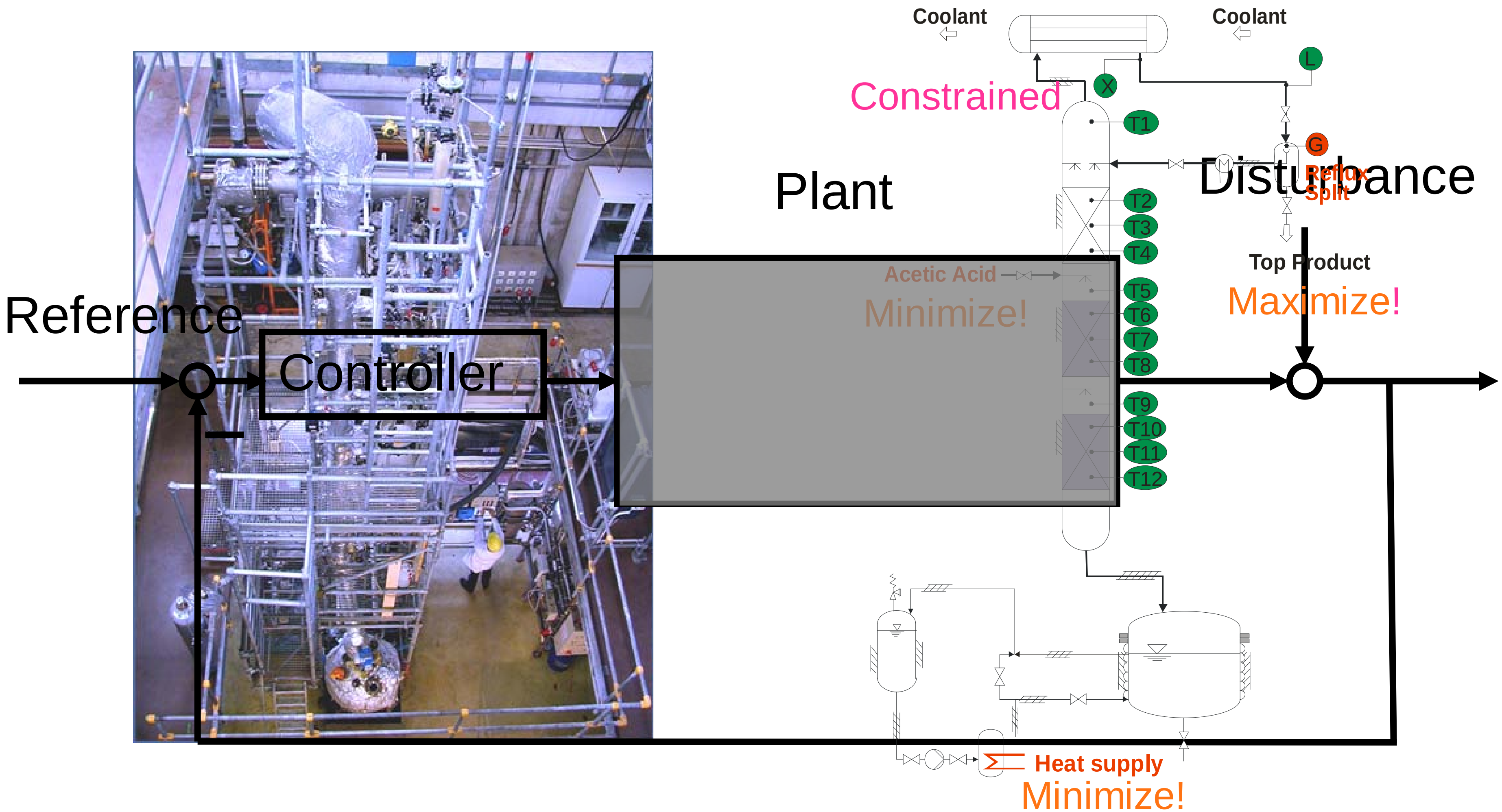
Process Operations



Reactive distillation column



Control Engineering Reduction



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”

- Servo problem formulation is mostly relevant 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

Control for Optimal Operation

✓ The gap between process control and process operations

- How to achieve near-optimal operation?
  - Regulatory control
  - Real-time optimization with regulatory control
- Direct finite-horizon optimizing control (DRTO)
- Application example: Chromatography
- Robustness
- Summary, open issues and future work

Plant Performance Based Control Structure Selection

- Discussed already by Morari, Stephanopoulos and Arkun (1980)
- 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

Comparison of Feedback Structures (Engell et al., 2005)

- 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)

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

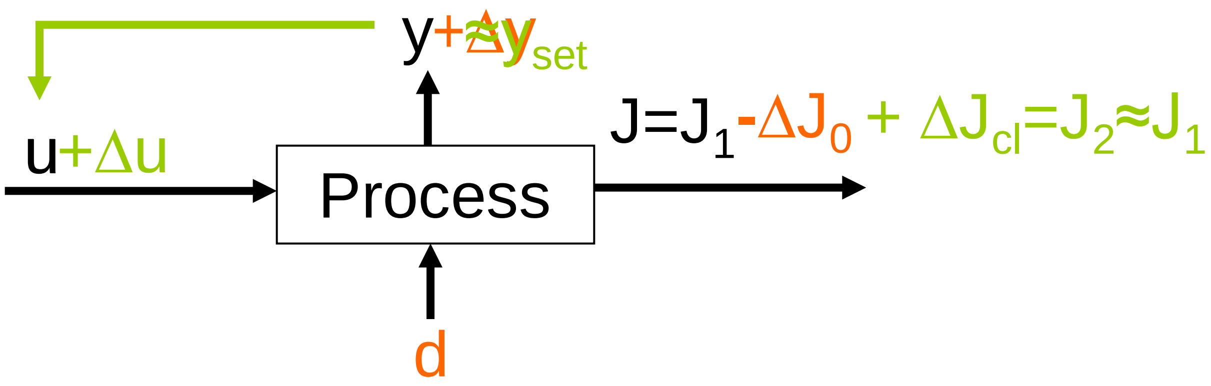
$$s.t.: \dot{\underline{x}} = \underline{f}(\underline{u}, \underline{d}_i, \underline{x}) = 0$$

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

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

- Set-points optimized separately for a set of disturbances

The Effect of Regulation on the Profit



$$\Delta J = J(\underline{u}_{nom}, d = 0) - J(\underline{u}_{nom}, \underline{d}_i) \quad (1)$$

$$+ J(\underline{u}_{nom}, \underline{d}_i) - J(\underline{u}_{opt}, \underline{d}_i) \quad (2)$$

$$+ J(\underline{u}_{opt}, \underline{d}_i) - J(\underline{u}_{con}, \underline{d}_i). \quad (3)$$

(1) ≈ 0:

No regulatory control necessary

(1) >> 0 and (2) << 0 and (3) ≈ 0:

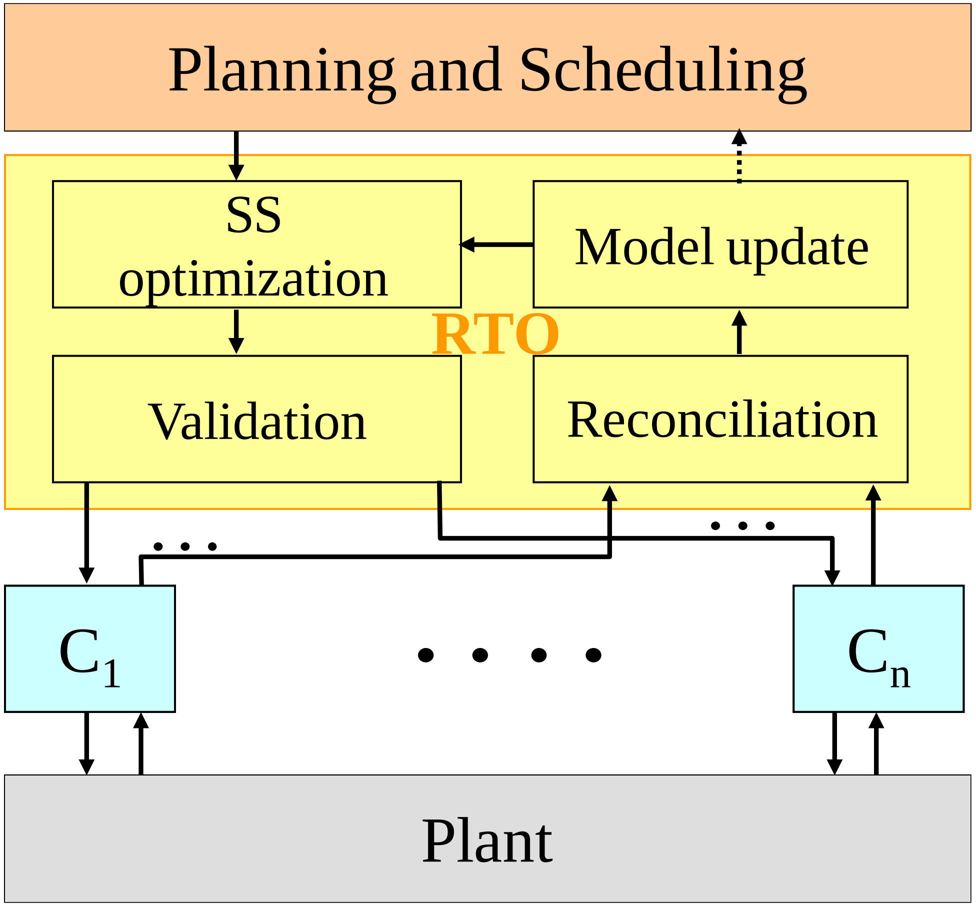
Closed-loop regulatory control recommended

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

Control with fixed set-point not advisable

RTO

- If regulatory control with fixed set-points is not good enough: RTO – real time optimization



Two-layer Architecture with RTO

- Online computation of optimal setpoints using nonlinear (mostly mechanistic) steady-state models (aka RTO)
- Realization of the setpoints by servo/regulatory control, using linear models (linear MPC or standard controllers)
- Optimization can only be performed after a steady state of the plant is confirmed

➡ Clear separation of concerns, but
  - Reaction to disturbances takes at least one settling time of the plant plus one settling time of the regulatory layer
  - Limited bandwidth, > 1/(***plant*** settling time)

RTO performance evaluation

- Loss of performance compared to the theoretical optimum (Forbes and Marlin,1996, Zhang and Forbes, 2000)
  - ***Bias*** – caused by model errors
  - ***Variance*** – caused by measurement errors
  - ***Steady-state*** optimization instead of dynamic optimization
- plus
  - ***Implementation*** errors (control layer does not realize the computed steady state)
- **Fair comparison** (Duvall and Riggs, 2000):
  Well-trained operators who know which variables should be at the constraints whereas the rest is controlled at fixed setpoints (→ self-optimizing control)

Real-time Optimization – Problems and Challenges

- Steady-state detection
- Model consistency between the layers
- Handling of hard constraints
  - Propagate to the control layer → infeasibility handling?
  - Implement as setpoints with safety margin
- Model accuracy (gradient and curvature of the cost function) → measaurement-based optimization
- Marlin and Hrymak (CPC 1996):
  - Tight integration of the design of RTO, result filtering, and implementation by feedback control necessary.
  - RTO should provide a controller design, not just setpoints.

From RTO to Dynamic Optimization

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

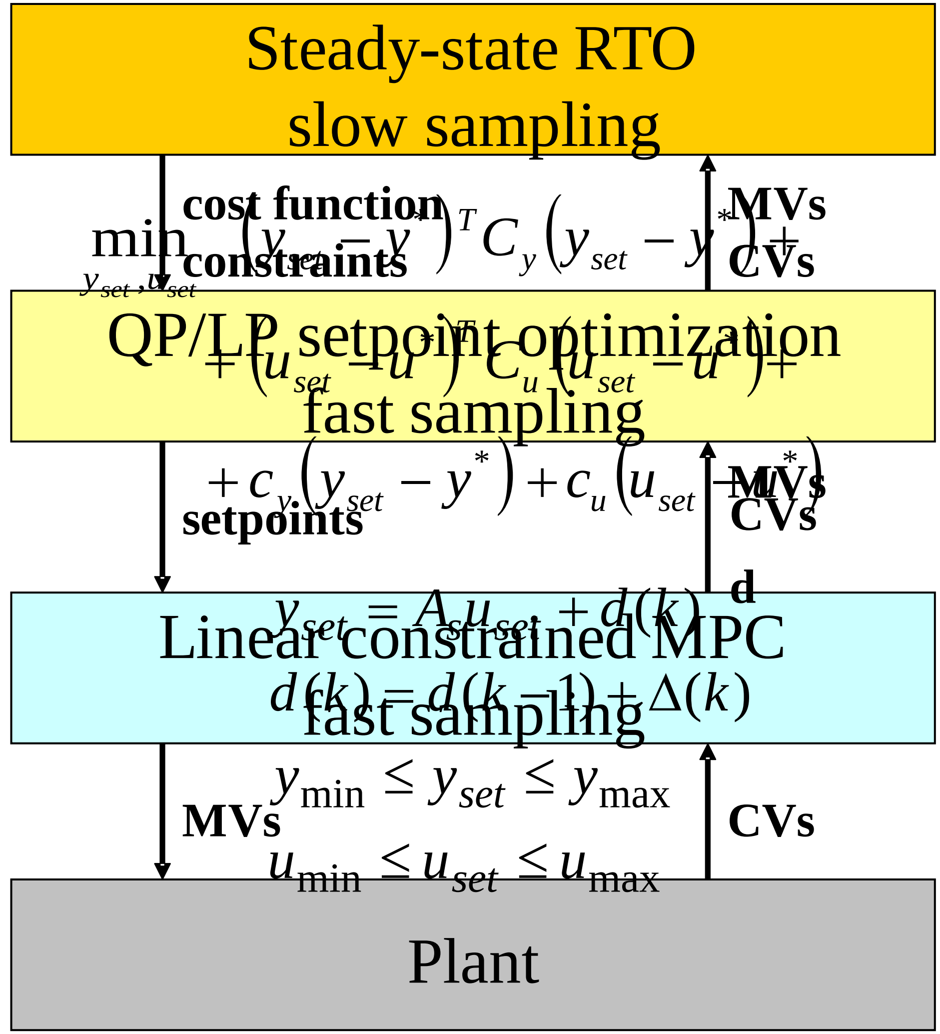
  hence
- Do not wait for steady state → ***fast sampling RTO***
  - Current industrial practice:

    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

Two layer MPC

- Optimization of the setpoints on an intermediate layer
  - based upon the same linear model as on the MPC layer
  - targets and weights provided by the RTO layer
  - disturbance estimate provided by the MPC layer
- ⇨ Improvement of dynamic response (smoother transients)
- ⇨ Enhanced stability (Ying and Joseph, 1999)



$$\min_{y_{set},u_{set}} \left(y_{set}-y^*\right)^T C_y \left(y_{set}-y^*\right) + \left(u_{set}-u^*\right)^T C_u \left(u_{set}-u^*\right) + c_y\left(y_{set}-y^*\right) + c_u\left(u_{set}-u^*\right)$$

$$y_{set} = A_s u_{set} + d(k)$$

$$d(k) = d(k-1) + \Delta(k)$$

$$y_{min} \le y_{set} \le y_{max}$$

$$u_{min} \le u_{set} \le u_{max}$$

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):

$$\min_{\Delta u(k+i);i=0,\ldots,m-1} \sum_{j=1}^{p} \left\| W_1 (y(k+j)-r) \right\|_2^2$$

$$+\sum_{i=0}^{m-1} \left\| W_2 \Delta u(k+i) \right\|_2^2 + W_3 f_{eco}(u(k+m-1))$$

$$+\left\| W_5 (u(k+m-1)-u(k-1)-\Delta u(k)) \right\|_2^2$$

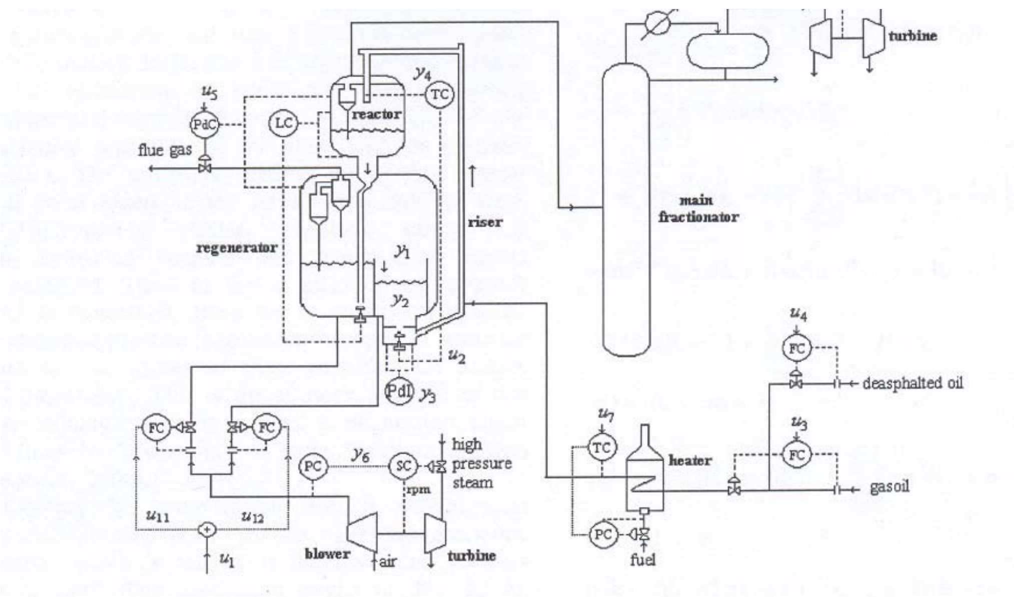
$$+W_6 [f_{eco}(u(k+m-1), y(k+\infty))$$

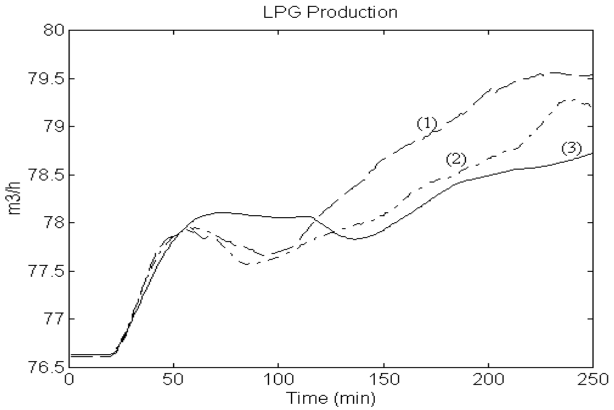
$$- f_{eco}(u(k), y'(k+\infty))]^2$$

Application to a Real Industrial FCC

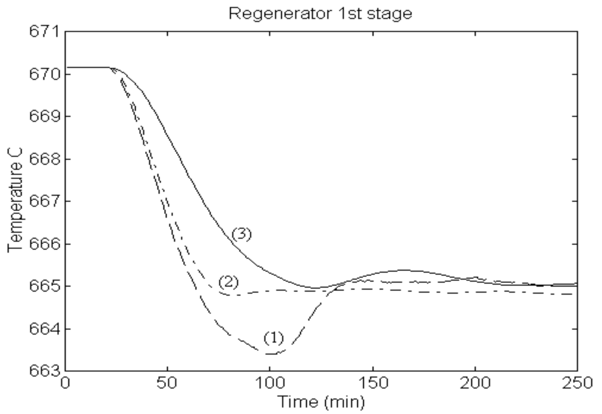
7/6 inputs, 6 outputs

Economic criterion: LPG-production





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



Problems: Acceptance by operators

Concerns for vulnerability

Control for Optimal Operation

- ✓ The gap between process control and process operations
- ✓ How to achieve near-optimal operation?
  - Regulatory control
  - Real-time optimization with regulatory control
- Direct finite-horizon optimizing control (DRTO)
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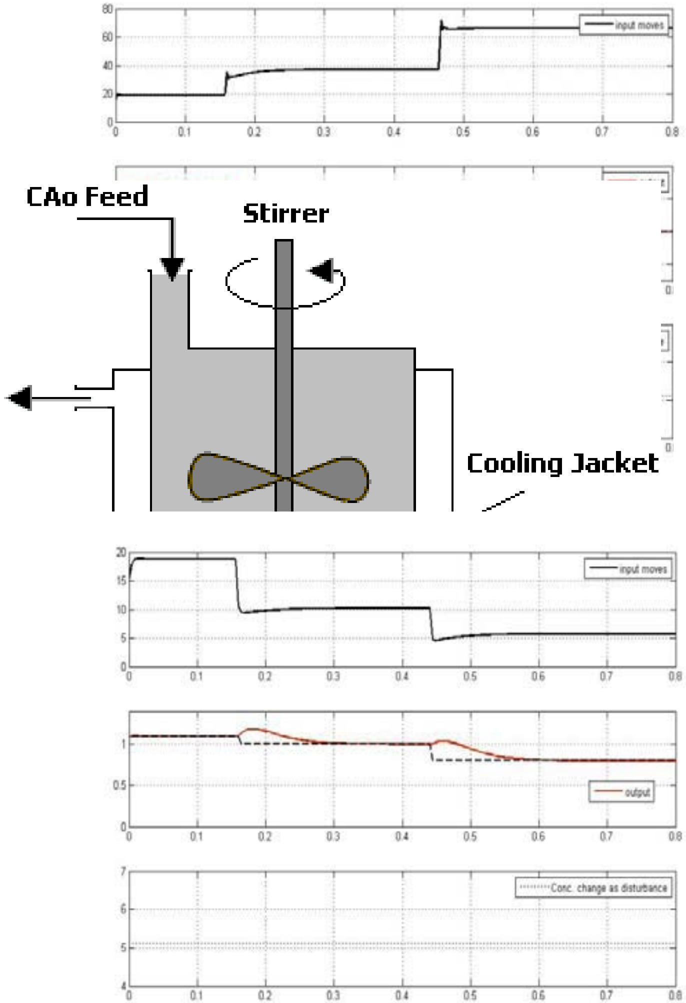
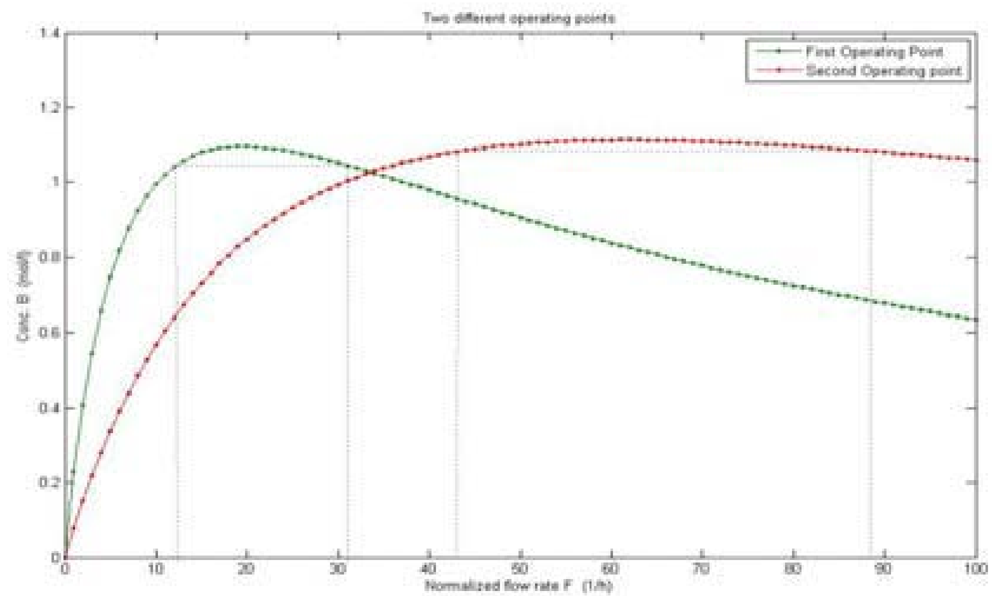
Direct Finite Horizon Optimizing Control

- Idea:
  - Optimize - over a finite moving horizon - the (main) degrees of freedom of the plant with respect to process performance rather than tracking performance using rigorous models
  - 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

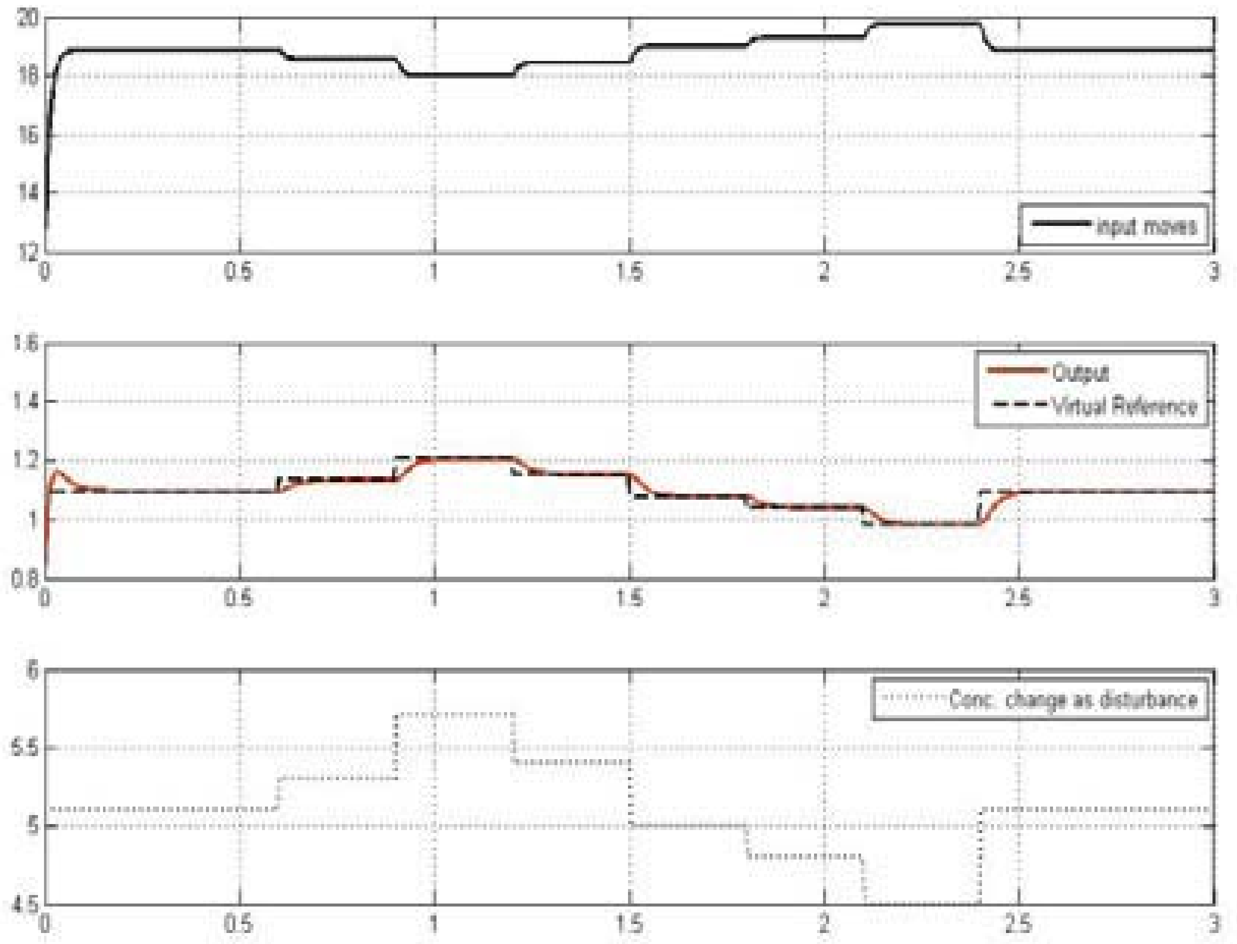
➡ Maximum freedom for economic optimization

Simple Example: CSTR with Unstable Zero Dynamics





Maximum Conversion by Optimizing Control

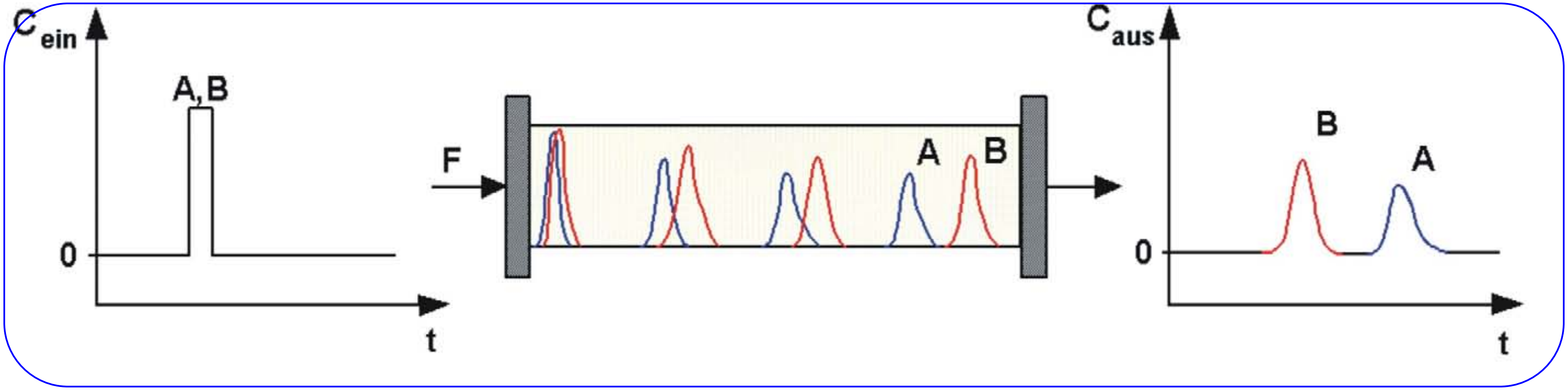


Direct Finite Horizon Optimizing Control

- 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: SMB Chromatography

Chromatography: Batch Process

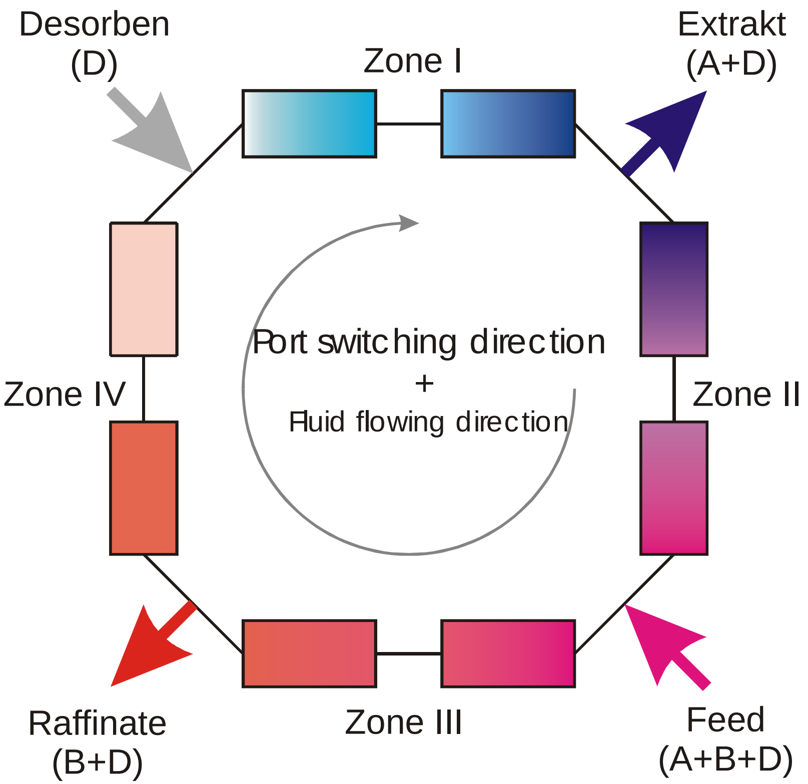


- Separation is based on different adsorption affinities of the components to a fixed adsorbent.
- Gradual separation while the mixture is moving through the column
- Fractionating of the products at the column outlet

☺ Simple process, high flexibility

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

Simulated-Moving-Bed Process

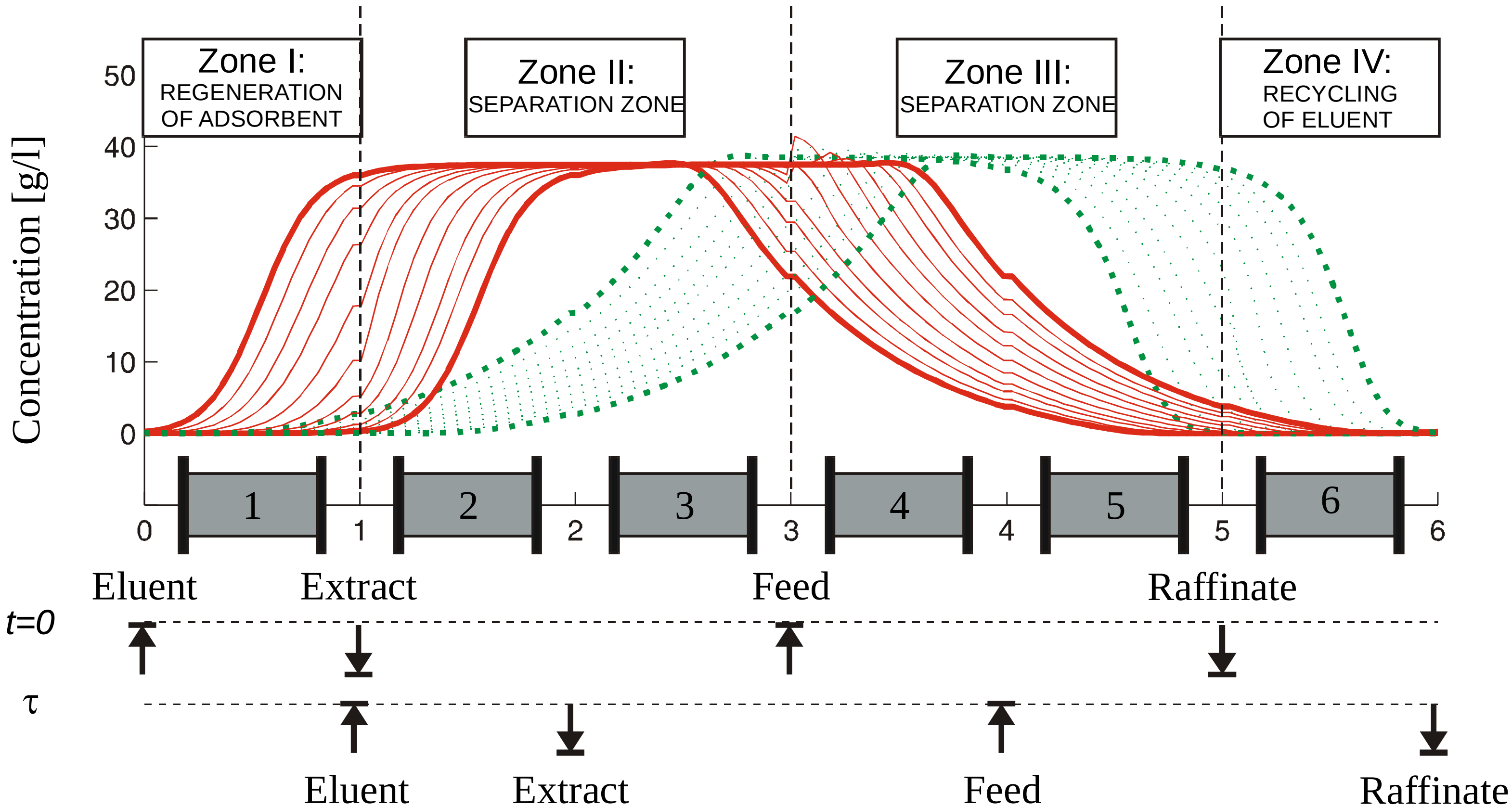


- A number of chromatographic columns are connected in series
- The inlet and outlet ports move to the next column position after each swichting period (τ)
- Quasi-countercurrent operation is achieved ("simulated") by cyclic port switching

☺ Continuous operation, higher productivity, and lower separation cost

☹ Complex dynamics, very slow reaction to changes

SMB Dynamics



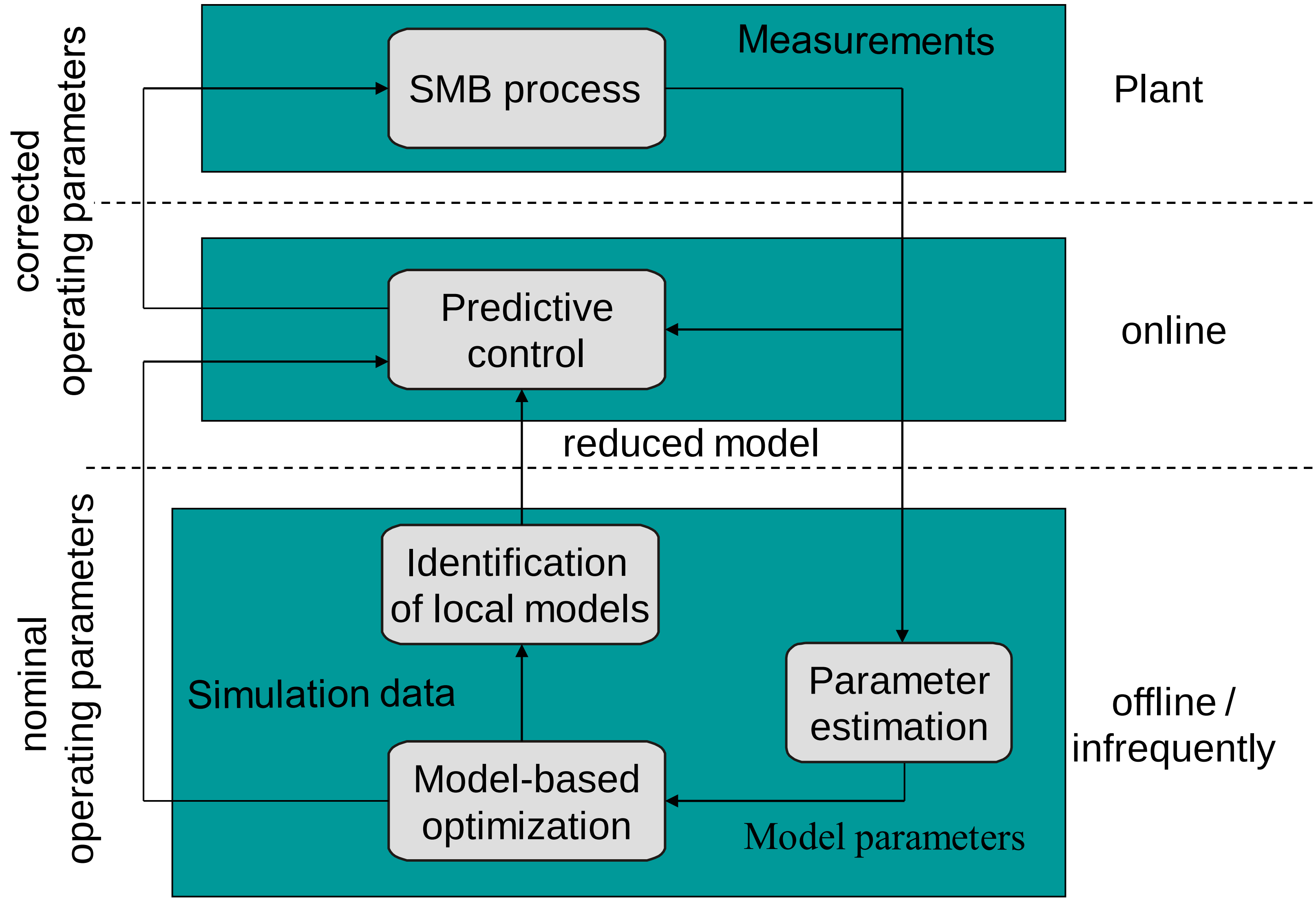
$$\mathbf{c}_{\mathbf{ax,k}}(t=\tau)=\mathbf{P}\mathbf{c}_{\mathbf{ax,k}}(t=0)$$

SMB Optimization and Control Problem

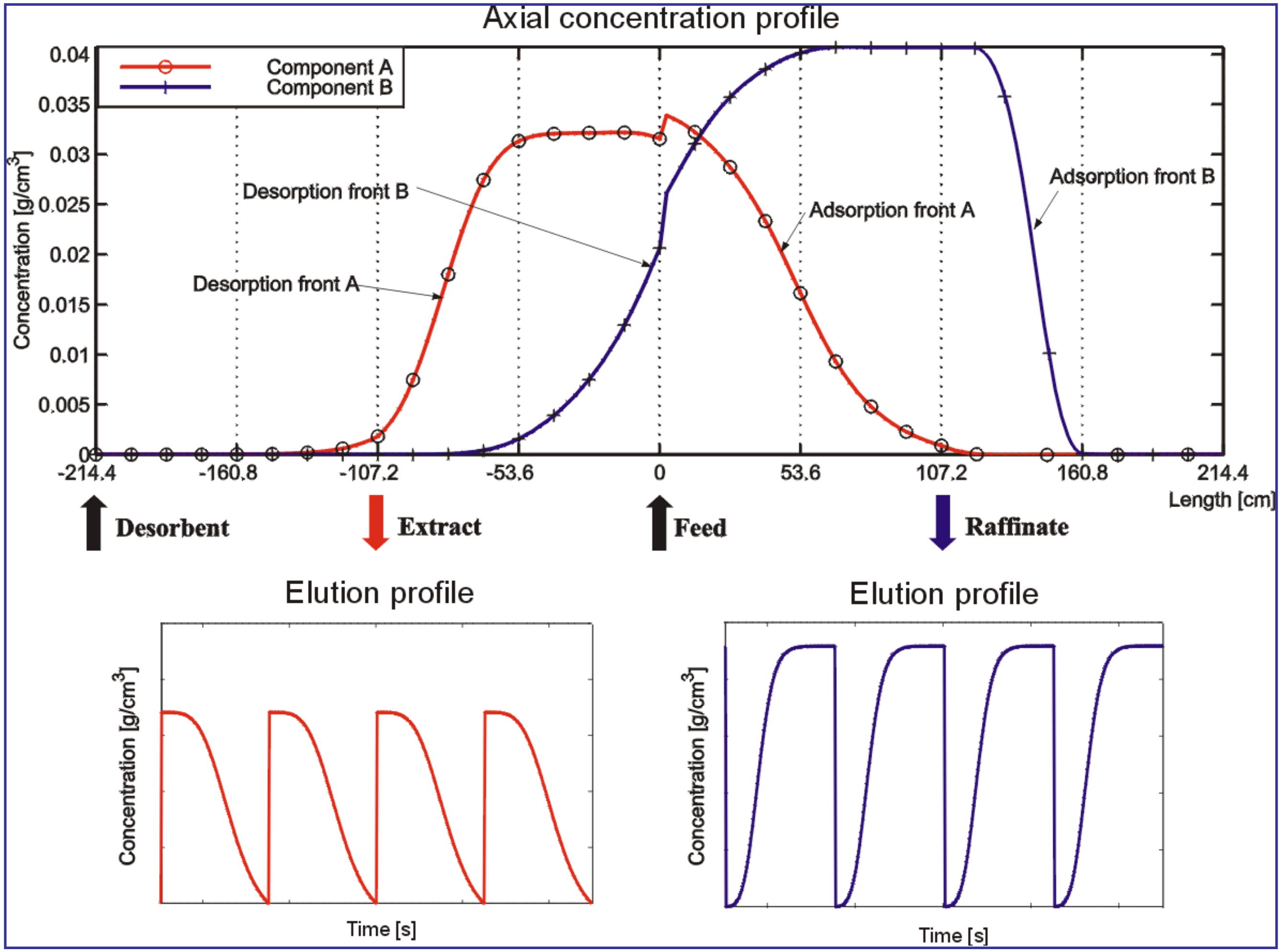
- **Goal:** Maintain specified purity at minimal operating cost
- Periodic process described by switched pde's
- Strongly nonlinear behaviour especially for nonlinear adsorption isotherms
- Drifts may lead to breakthrough of the separation fronts → long periods of off-spec production
- Intuitive determination 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.)



Low-level control: Front stabilization

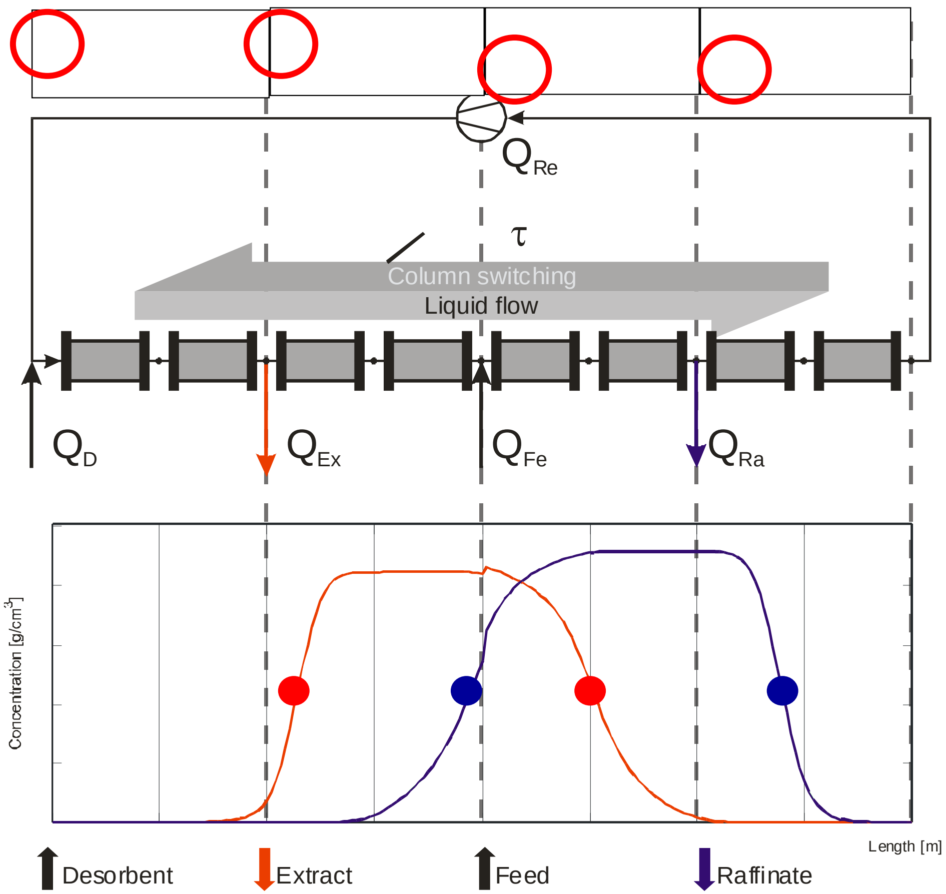


Stabilising the concentration profile

- 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

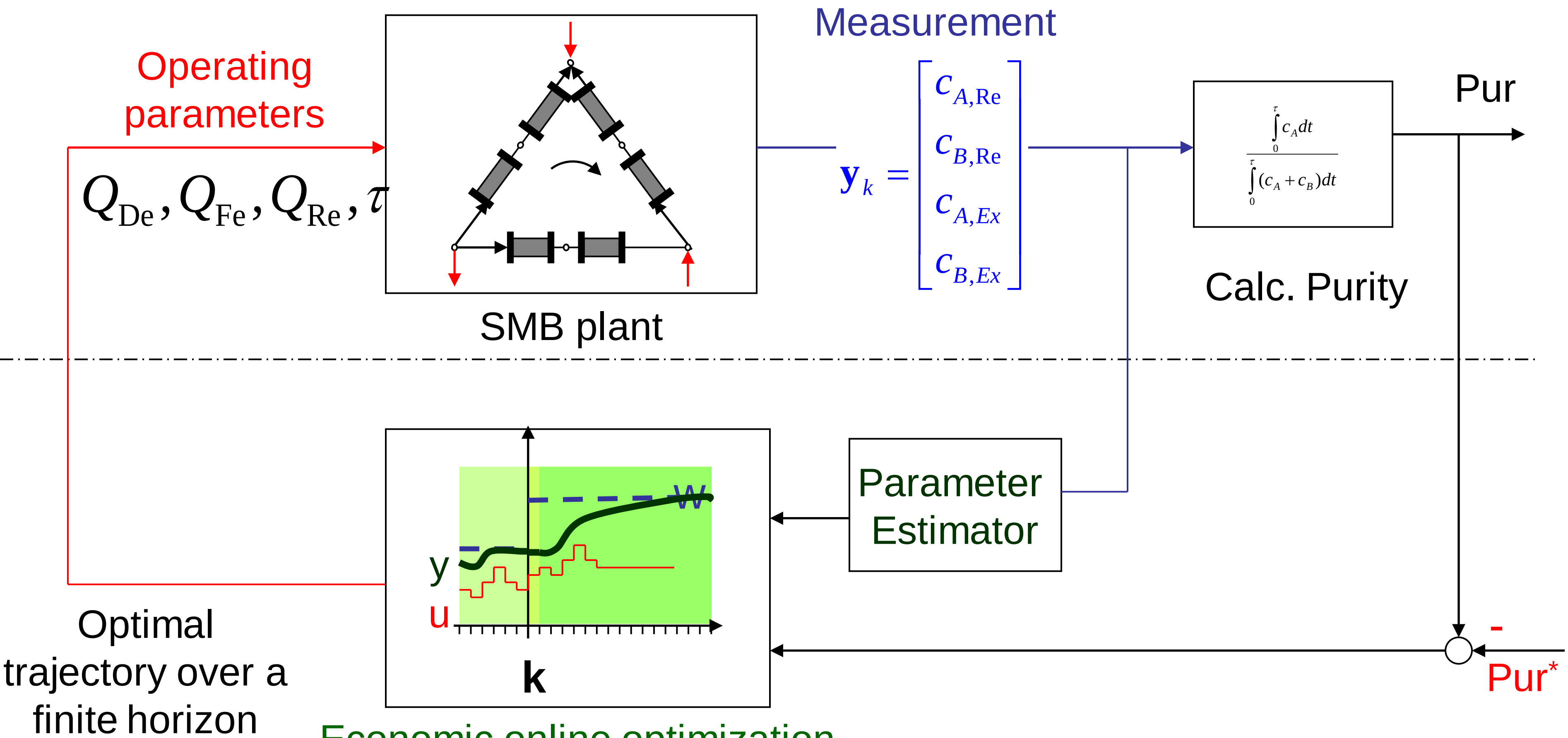
- Extension to nonlinear isotherms possible but control scheme quite complex (NN-based LPV MPC) (Wang and Engell, 2003)
- Fronts can only be detected accurately in the recycle stream, not in the product streams
- Optimality and desired purities cannot be guaranteed by front position control if the model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

  →additional purity control layer necessary

  →Scheme becomes very complex, optimality is lost.

⇨ Use online optimization directly to control the plant!

Moving horizon optimizing control



Economic online optimization based upon a full nonlinear model

Toumi & Engell, Chem. Eng. Sci. 2004
similar work at ETH Zürich

Control by Online Optimization

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

Θ: economic criterion: solvent consumption

β_k degrees of freedom – transformed flow rates and switching time

s.t.

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

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

$$j = k,..,k + H_p$$

Features of the Control Strategy

- The usual control variable (purity) appears as a constraint and a cost function is minimised.
- Structural plant-model mismatch handled by additive updated purity disturbance.
- To reduce plant-model mismatch, the model is adapted periodically by solving a least squares problem with respect to selected sensitive parameters.
- Numerical solution: sequential approach
  - Simulation to the cyclic steady state
  - Small number of degrees of freedom
  - Feasible path SQP-solver FFSQ
  - Optimisation stopped when the sampling period is exceeded

Mathematical modelling: Full model

Hybrid Dynamics

- Node Model (change in flow rates and concentration inputs)
- Synchronous switching (new initialization of the state)
- Continuous chromatographic model (*General Rate Model*)

$$\frac{\partial c_i}{\partial t}+\left(\frac{1-\varepsilon_b}{\varepsilon_b}\right)\frac{3k_{l,i}}{r_p}\left(c_i-c_{p,i}|_{r=r_p}\right)=D_{ax,i}\frac{\partial^2 c_i}{\partial x^2}-u\frac{\partial c_i}{\partial x},$$

$$(1-\varepsilon_p)\frac{\partial q_i}{\partial t}+\varepsilon_p\frac{\partial c_{p,i}}{\partial t}-\varepsilon_p D_{p,i}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial c_{p,i}}{\partial r}\right)\right]=0,$$

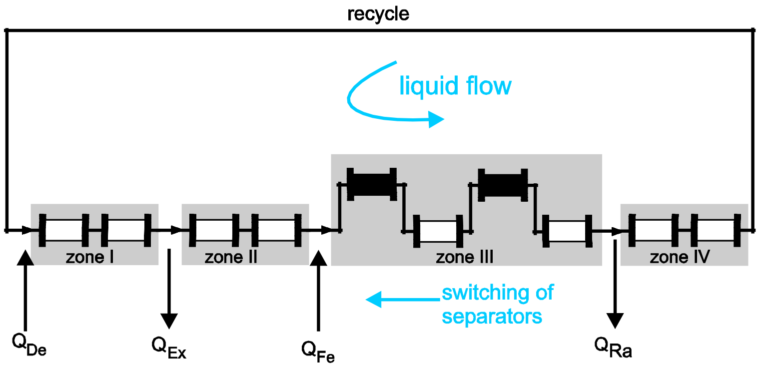
$$q_i=f(c_{p,1},\cdots,c_{p,nsp}).$$

Numerical approach (Gu, *1995,* Toumi)

- Finite Element discretisation of the fluid phase
- Orthogonal Collocation for the solid phase
- ⇨ stiff ordinary differential equations solved by lsodi (Hindmarsh et al.)
- ⇨ Efficient and accurate process model (672 state variables for $\boldsymbol{n_{elemb}}$=10, $\boldsymbol{n_c}$=1, $\boldsymbol{N_{col}}$=8)

Reactive SMB Process

- 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

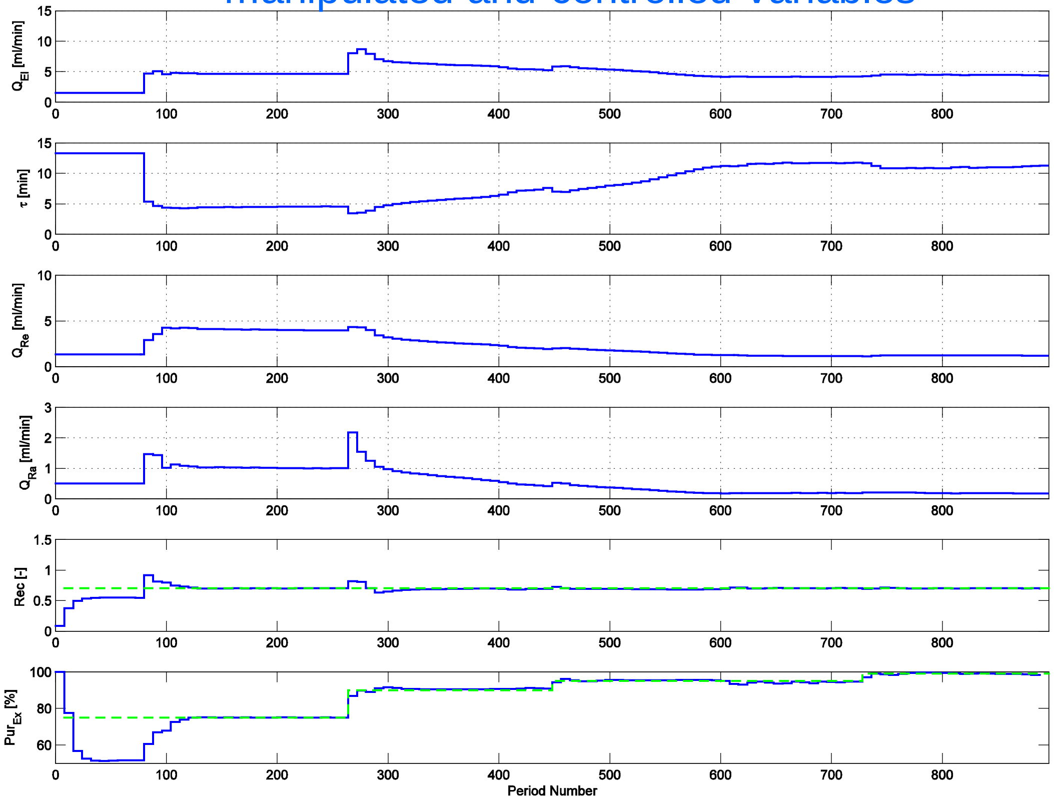
Simulation of the Optimizing Controller

- Purity and recovery constraints enforced
- Plant/model mismatch

(H_A +10%, H_B -5%)

- Controller reduces the solvent consumption
- Satisfaction of process requirements

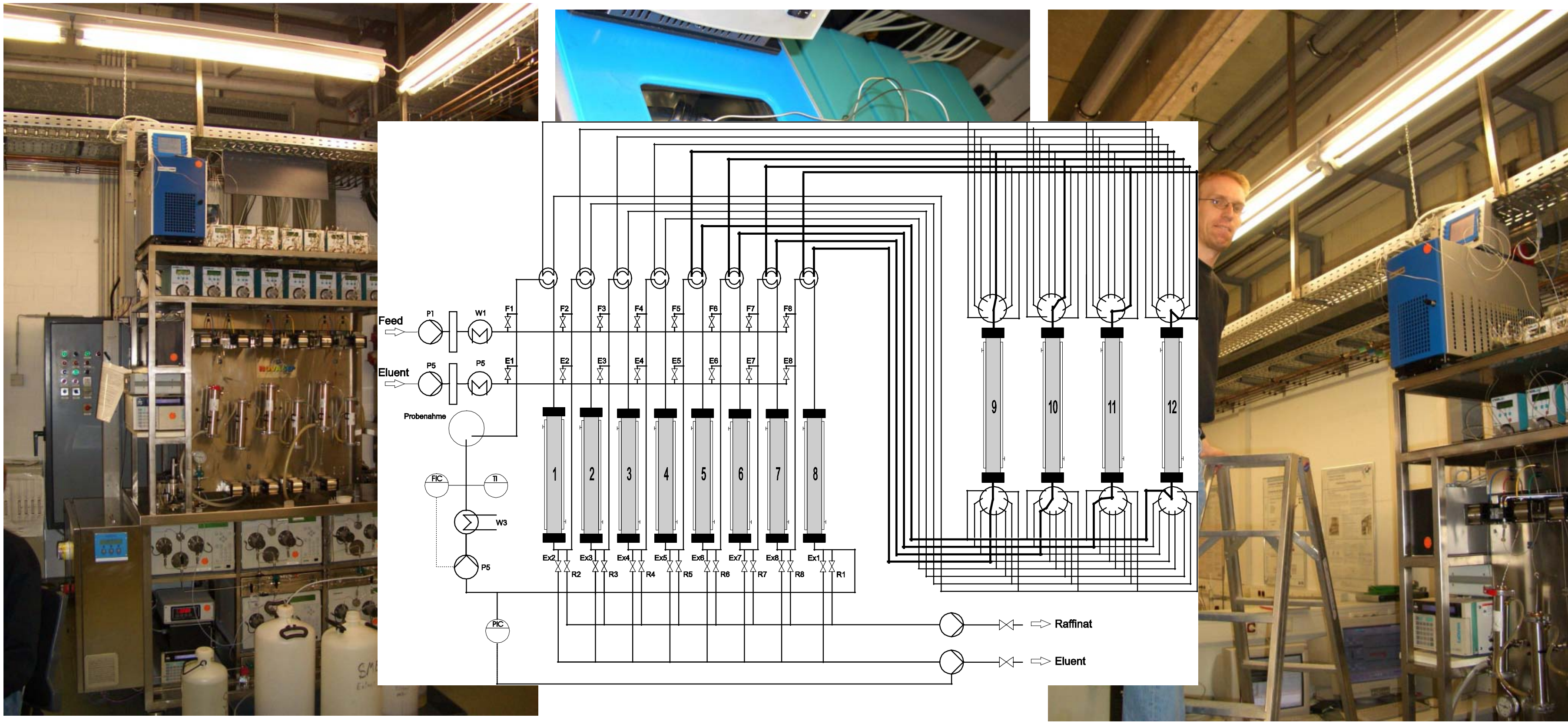
manipulated and controlled variables



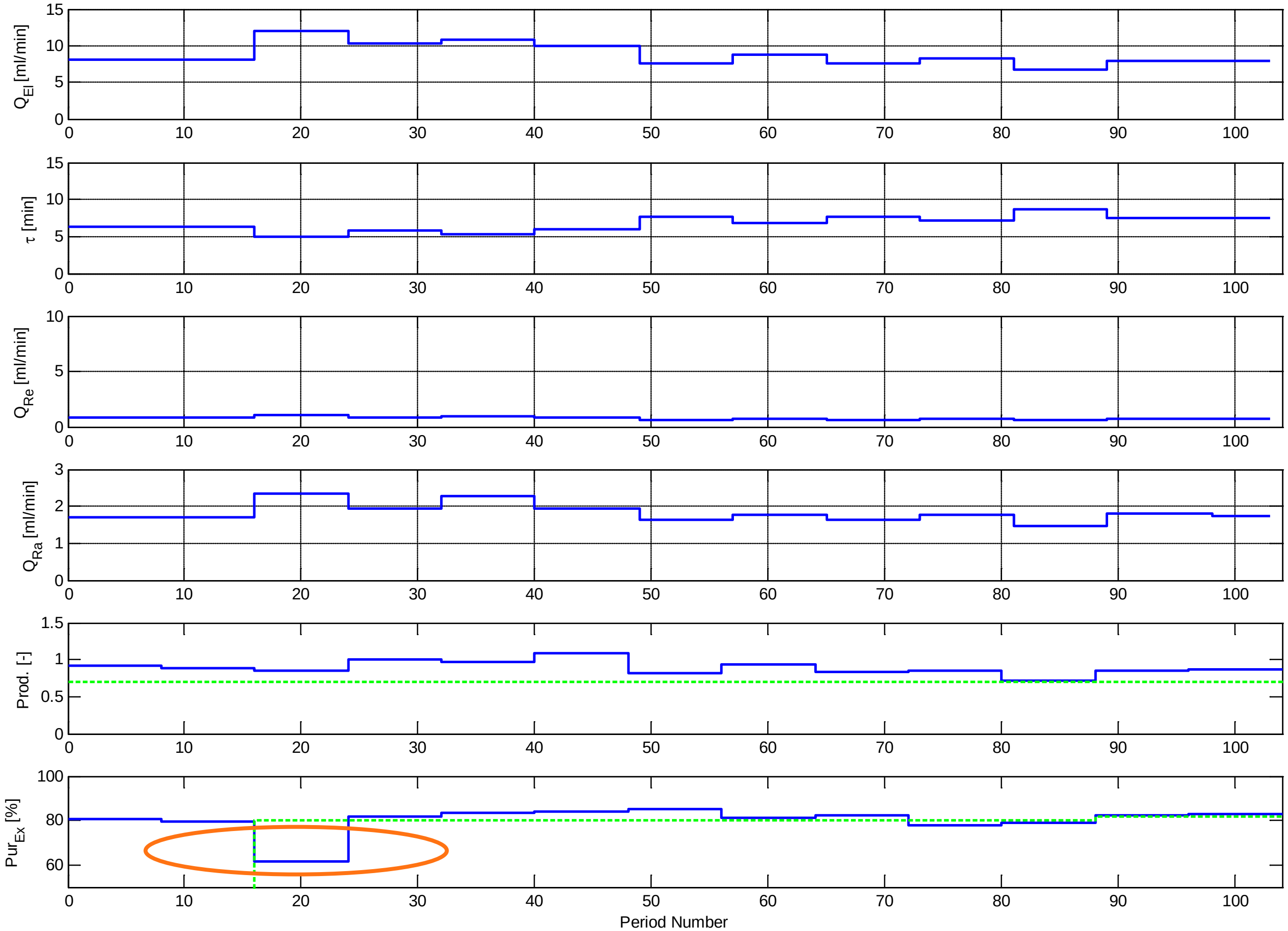
Technical Details

Sampling time	8 switching periods = 1 cycle
Prediction horizon	3 cycles
Control horizon	1 cycle
Controller start	2nd cycle
# state variables	1400
Degrees of freeedom (optimizer)	4 β-factors (corresponding to Q_i,, τ)
ode solver	DVODE
Optimizer	FFSQP
Computation time	Convergence achieved within 3 -6 switching periods

Experimental Hashimoto SMB Reactor



Experimental Results



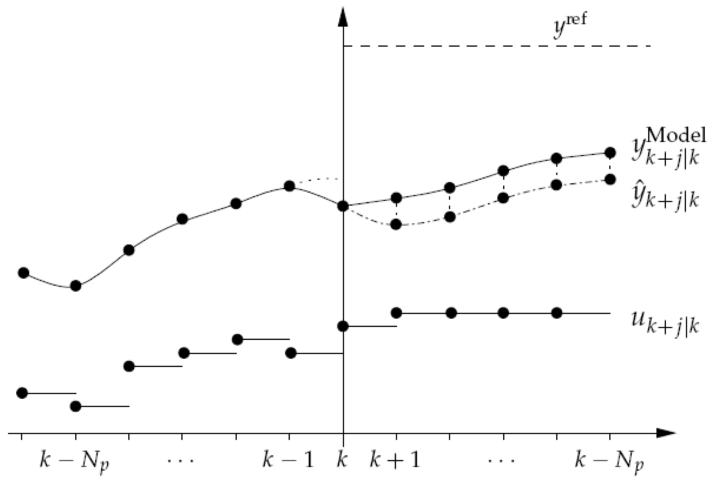
Violation of the purity constraint
because of a pump failure

Conclusion from the Case Study

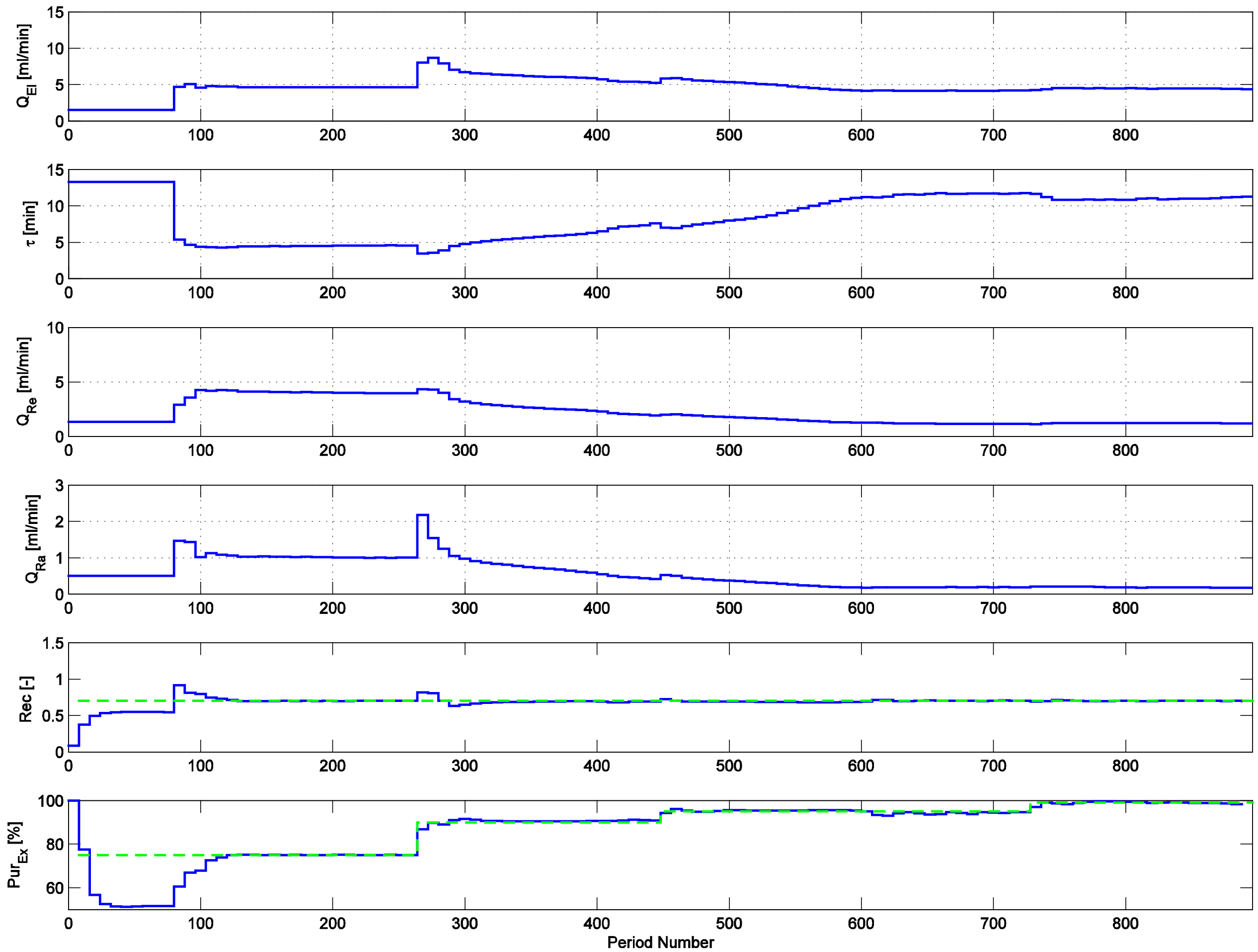
- Direct optimizing control is feasible and gives good results!
- Numerical aspects:
  - New general-purpose NLP algorithms for dynamic problems provide sufficient speed for faster processes (Biegler et al., Bock et al.)
  - Special algorithms taylored to online control for short response times (~ s) (real-time iteration, 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 ...**

NMPC and Model Accuracy

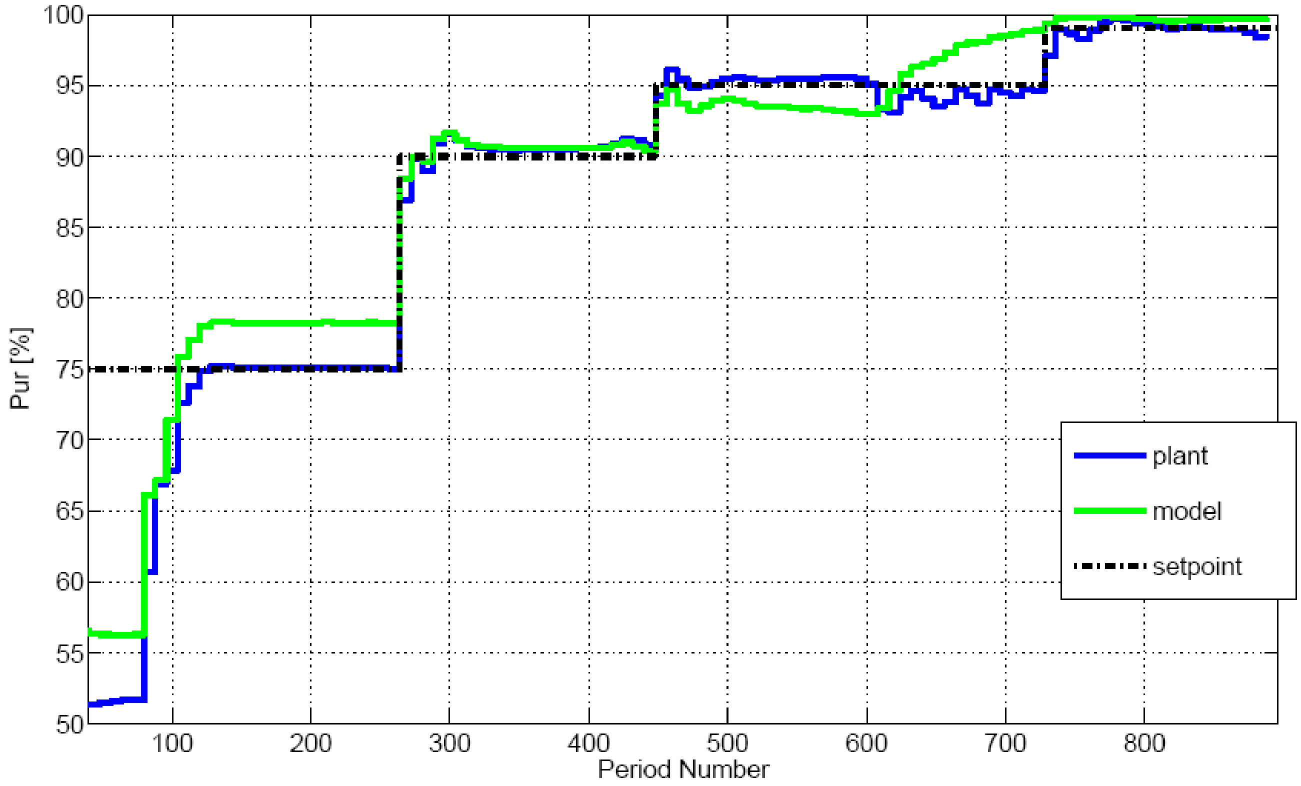
- The idea of (N)MPC is to solve a forward optimization problem repeatedly
- Quality of the solution depends fully on the model accuracy
- Feedback only enters by re-initialization and error correction (disturbance estimation) term
- Model errors are usually taken into account by a constant extrapolation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



Simulation of the Optimizing Controller



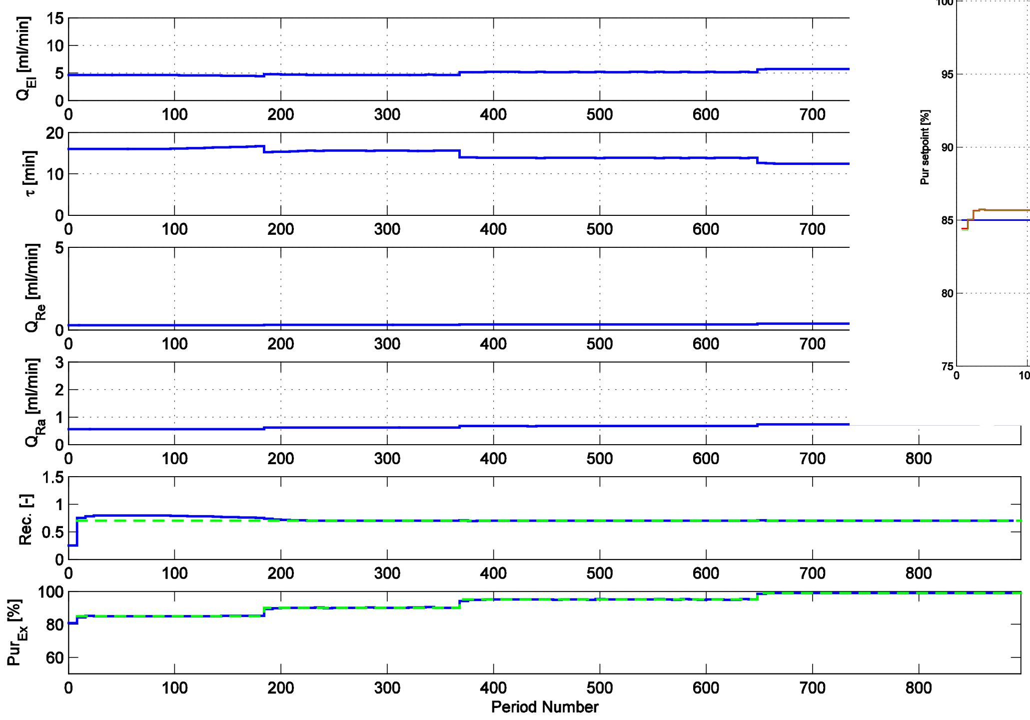
Plant-model Mismatch for Hashimoto SMB

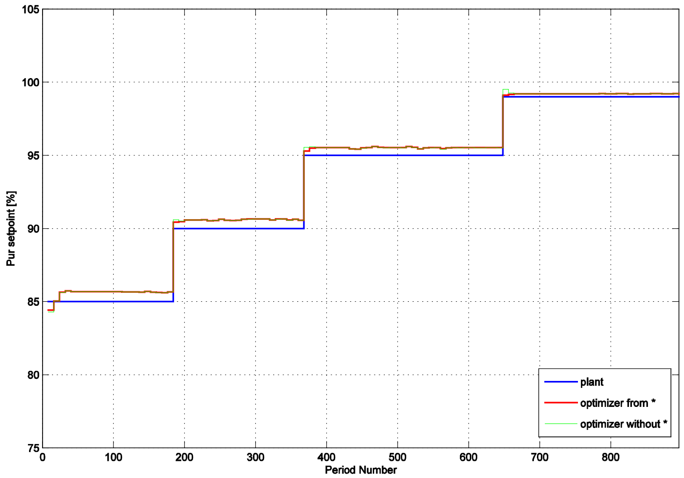


Modification of the Cost Function

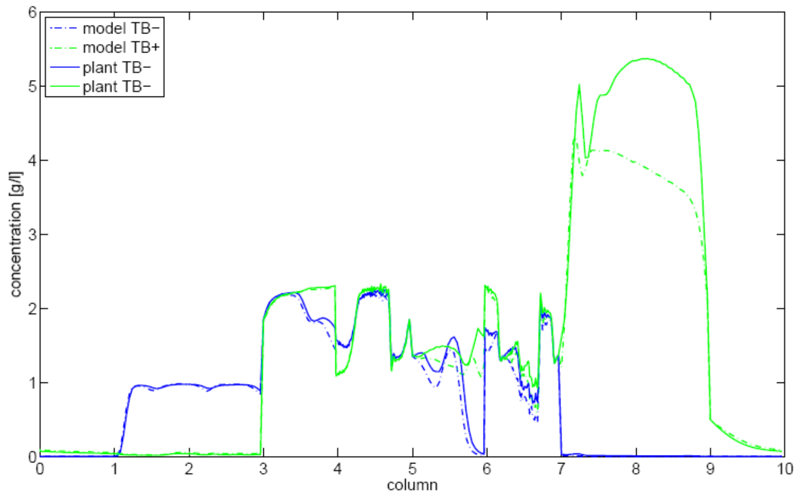
- Penalty term for breakthrough maintains standard operation
- Same simulation experiment as before

manipulated and controlled variab





Two Different Strategies



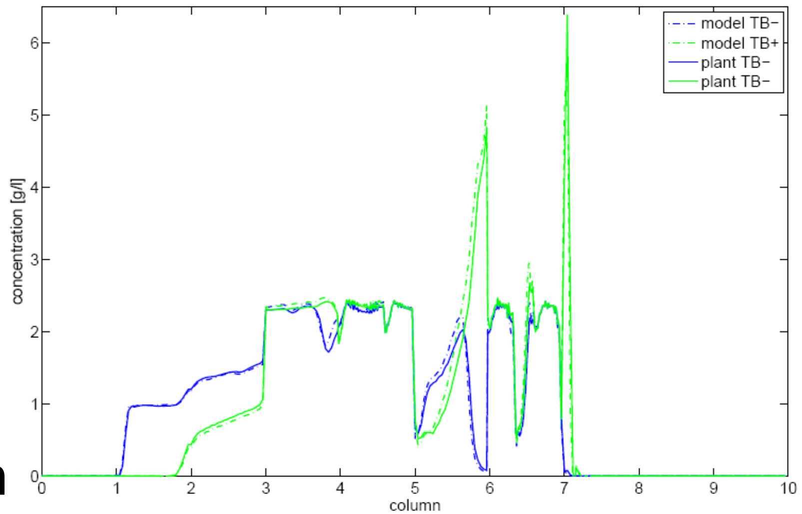
$$\min \sum_{j=k}^{k+H_p} (\Theta(j) + \Delta\beta_j{}^T R_j \Delta\beta_j)$$

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?

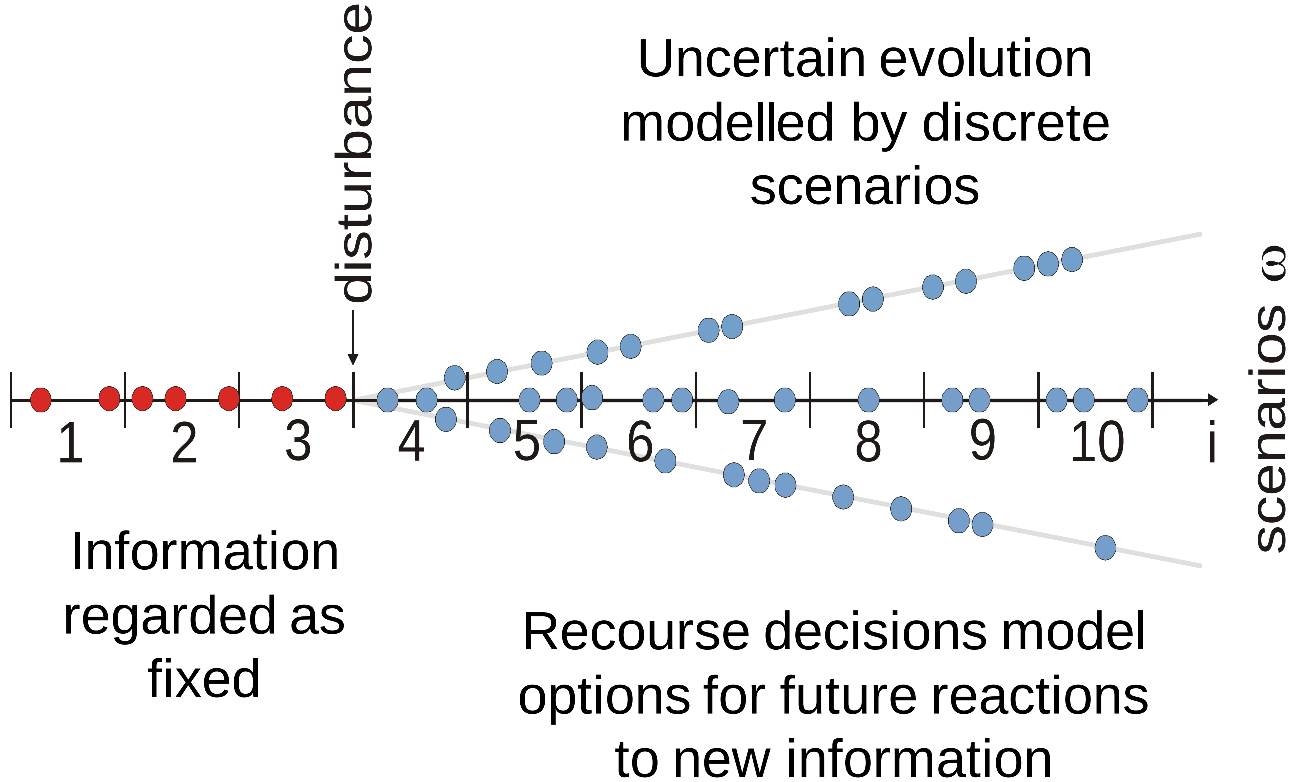
- Improve the quality of the model by parameter estimation
  - Numerical effort
  - Insufficient exitation during nominal operation
  - Structural plant-model mismatch

- 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)



Application to Robust NMPC

- Scenarios represent different models
- Next few inputs must work for all models
- BUT: After a difference between model and reality has been observed, the controller will react to it

⇨ Future inputs can be scenario dependent

  - Decisions are divided into “here and now” and “recourse”
  - **Optimistic approach: Correct model is revealed**
- **Alternatives:**
  - Only feasibility ensured
  - Optimization of the expected performance with recourse

Control for Optimal Operation

- ✓ The gap between process control and process operations
- ✓ How to achieve near-optimal operation?
  - Regulatory control
  - Real-time optimization with regulatory control
- ✓ Direct finite-horizon optimizing control (DRTO)
- ✓ Application example: Reactive chromatography
- ✓ Robustness
- Summary, open issues and future work

Summary

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

  ➡ ***Direct finite horizon optimizing control***

- **Main advantages*:***
  - Performance (see e.g. Ochoa et al., ADCHEM 2009)
  - 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.

	Steady-state performance	Dynamic performance	Stability	Numerical effort	Complexity of the formulation	Complexity for the operators	Vulnerability/ effort for safety
Direct optimizing control	++	**++**	?	very high	**low**	*high*	*high*
RTO + MPC	++/+	+	+	high	high	high	medium
RTO with linear control	+	0	?	high	low	medium	medium
Conventio-nal control	- → +	0	+	none	low	low	low

Open Issues

- **Modelling**
  - Dynamic models are expensive
  - Faithful training simulators are now 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
  - Infinite horizon?

More Research Topics

- Measurement-based optimization ➡ hints in the paper
- Constraint handling in case of infeasibility
- Reduction of complexity – (approximate) NCO tracking
  - Maximization of the throughput (Aske et al., IFAC ADCHEM 2009)
  - Maximizing the feed rate in batch processes online by feedback control
- Control architectures – decentralization, coordination

- **Key issues for real implementations:**
  - Operator interface
  - Plausibility checks, safety net