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Fakultät Bio- und Chemieingenieurwesen

Robust Optimizing Control of Chemical Processes

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D Y N

Outline

- Motivation for robust optimizing control
- Industrial reactor example
  - A simple optimizing control scheme
- Model-based optimizing control
  - Online state and parameter estimation with simplified models
  - Online optimization
- Multi-stage optimizing control
  - Idea and problem formulation
  - Results for a case study
- Summary, limitations and further work

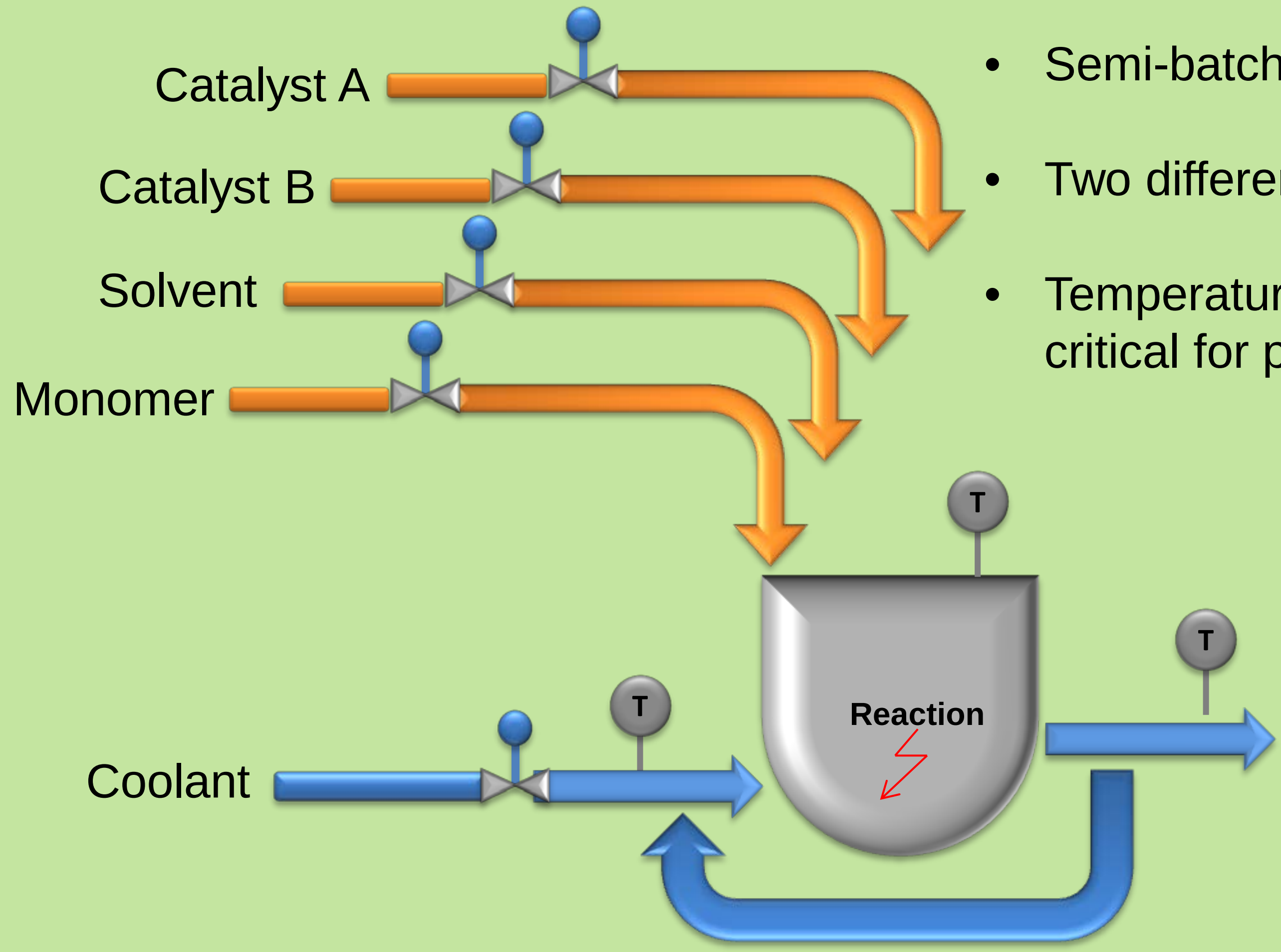
Motivation for robust optimizing control

- Operational excellence
  - Optimal utilization of equipment and resources
  - Minimization of unplanned shut-downs
  - Meeting of quality standards without re-work
  - Energy efficiency
  - Resource efficiency
- Operations in the process industries are subject to significant uncertainties
  - Changing process behaviours (e.g. catalyst efficiency)
  - Changing equipment
  - Changing feeds
  - External influences as e.g. outside temperature
- **Efficient, safe and reliable operation requires reactive measurement-based optimization**

Available technologies

- Feedback control to track given set-points
  - Requires a margin around the constraints
  - Set-points must be chosen well
- Optimization of set-points and high-quality control (RTO plus MPC)
- Model-based optimizing control:
  - The target of the controller is an economic optimization under constraints:
    - Safety limits
    - Product quality constraints
    - Equipment limitations
  - Depends critically on the accuracy of the model that is employed.

Example: Industrial polymerization process



- Semi-batch operation
- Two different products
- Temperature control is critical for product quality

Project funded by

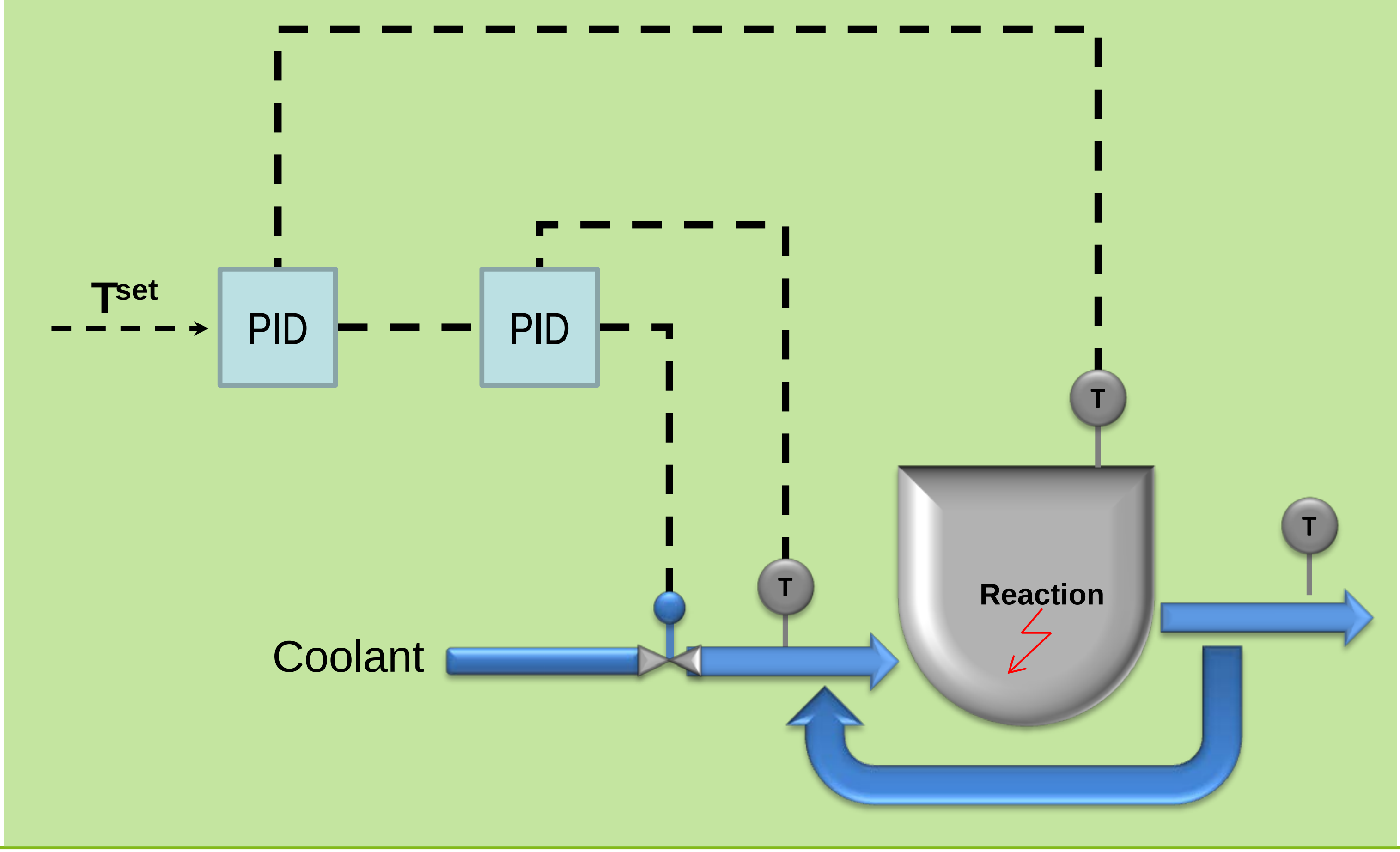
Ziel2.NRW
Regionale Wettbewerbsfähigkeit und Beschäftigung

- Goal:
  - Demonstrate that advanced control can be used for the improvement of the operation of a real polymerization reactor

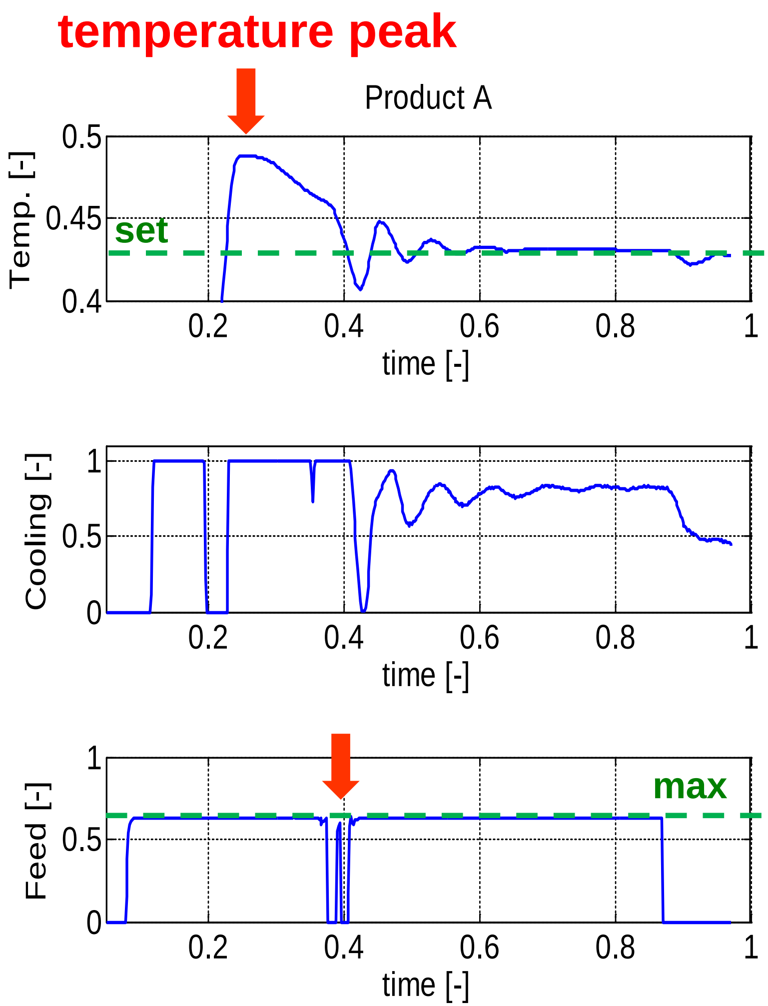
- Project Partners:
  - Evonik Industries
  - Leikon GmbH (Germany)
  - Process Dynamics and Operations Group (TU Dortmund)

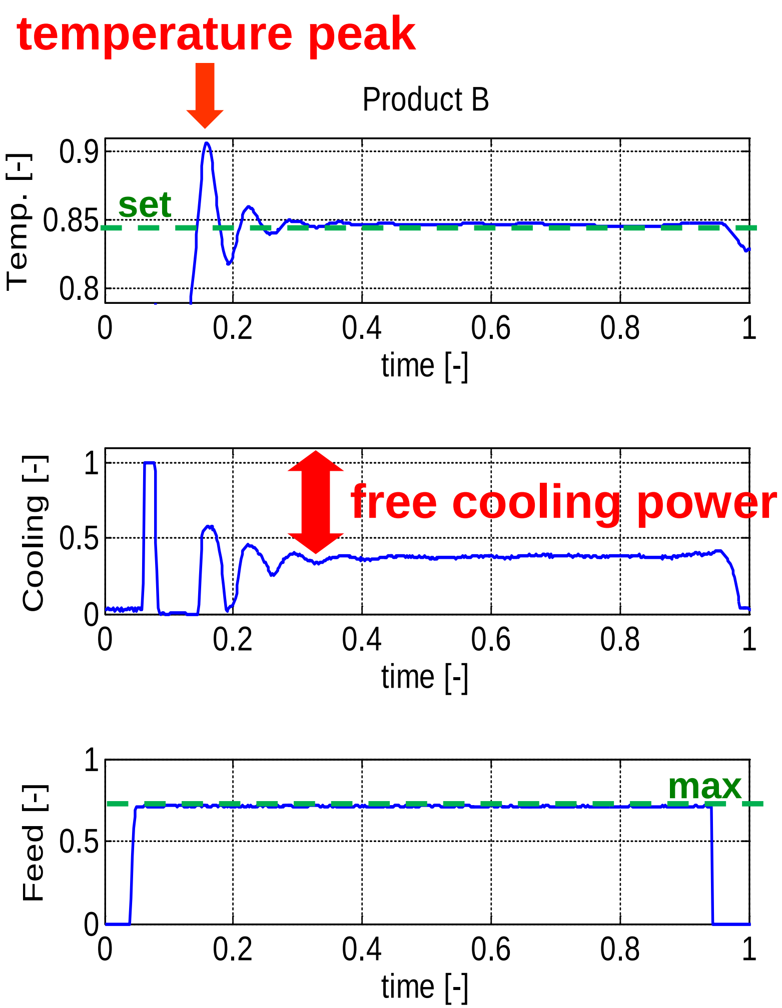
Starting point

- Manual setting of the monomer feed rate
- Cascaded temperature control



Batch runs with the standard structure





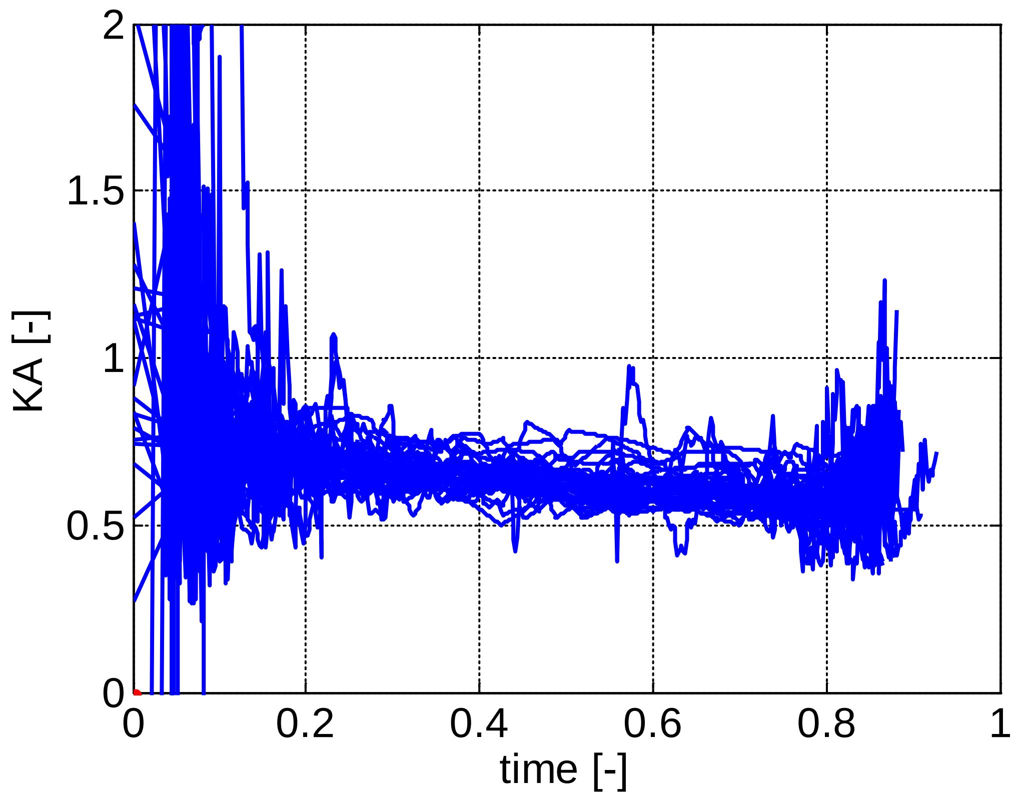
Goal and first step

- Development of an advanced control solution that optimizes the setting of the coolant flow and the monomer feed rate for
  - Improvement of the temperature control
  - Increase of the productivity (shorter batch times)

- It all starts with modelling …

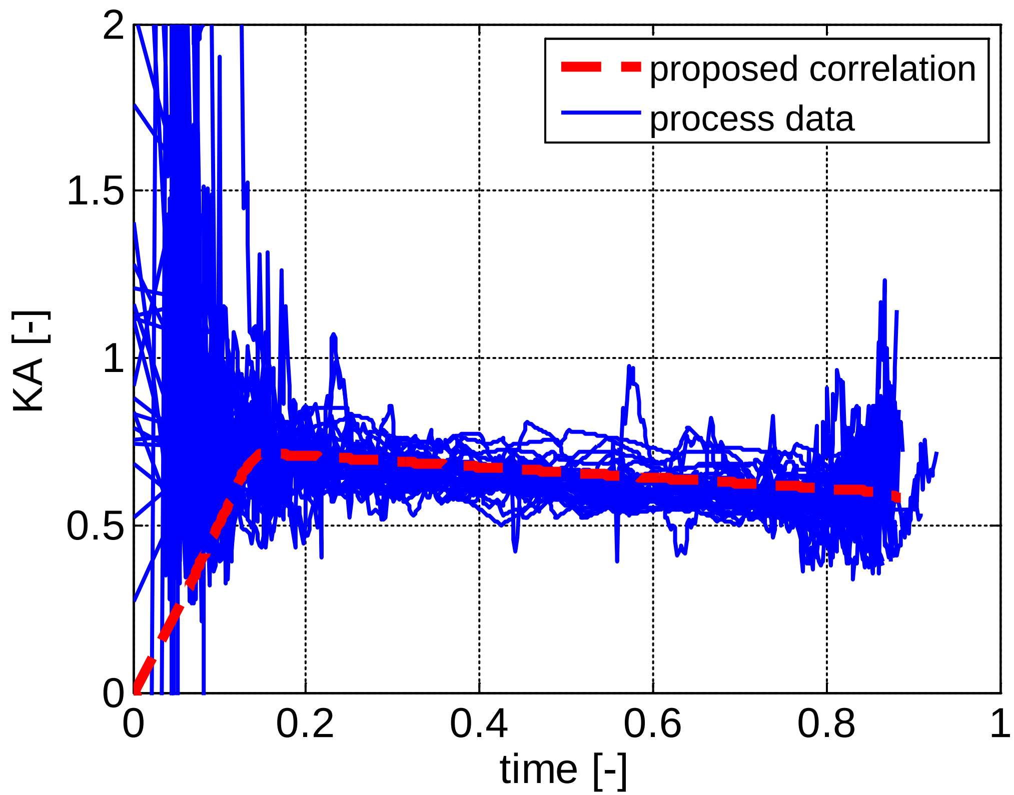
- Standard polymerization reactor model
  - Energy and mass balances
  - Reaction mechanism available in the literature
  - Equations for reaction rates, heat transfer coefficient, cooling power
  - Model for polymer chain growth

Empirical correlation for KA



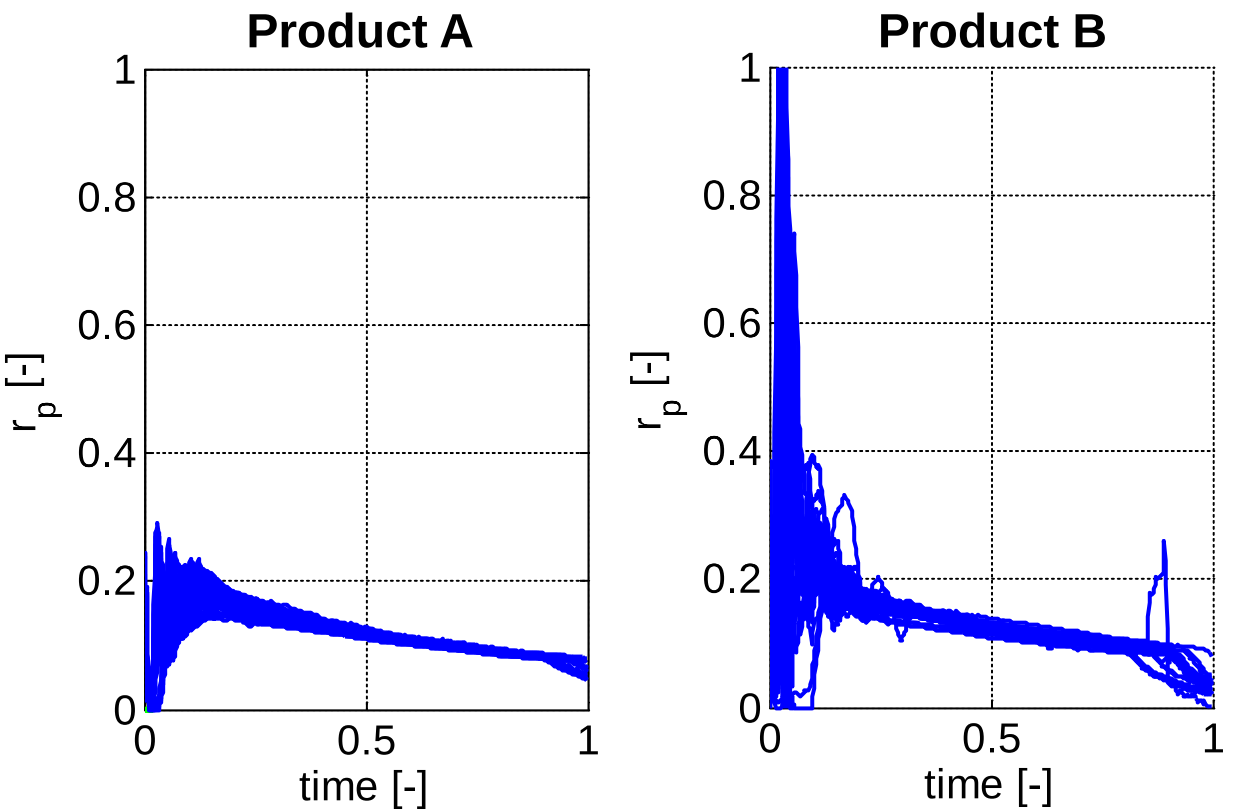
$$KA = \frac{CP_J M_J \frac{dT_J}{dt} - F_{cool} CP_W \left(T_{cool} - T_{J_{out}}\right)}{\left(T_R - T_J\right)}$$

Empirical correlation for KA



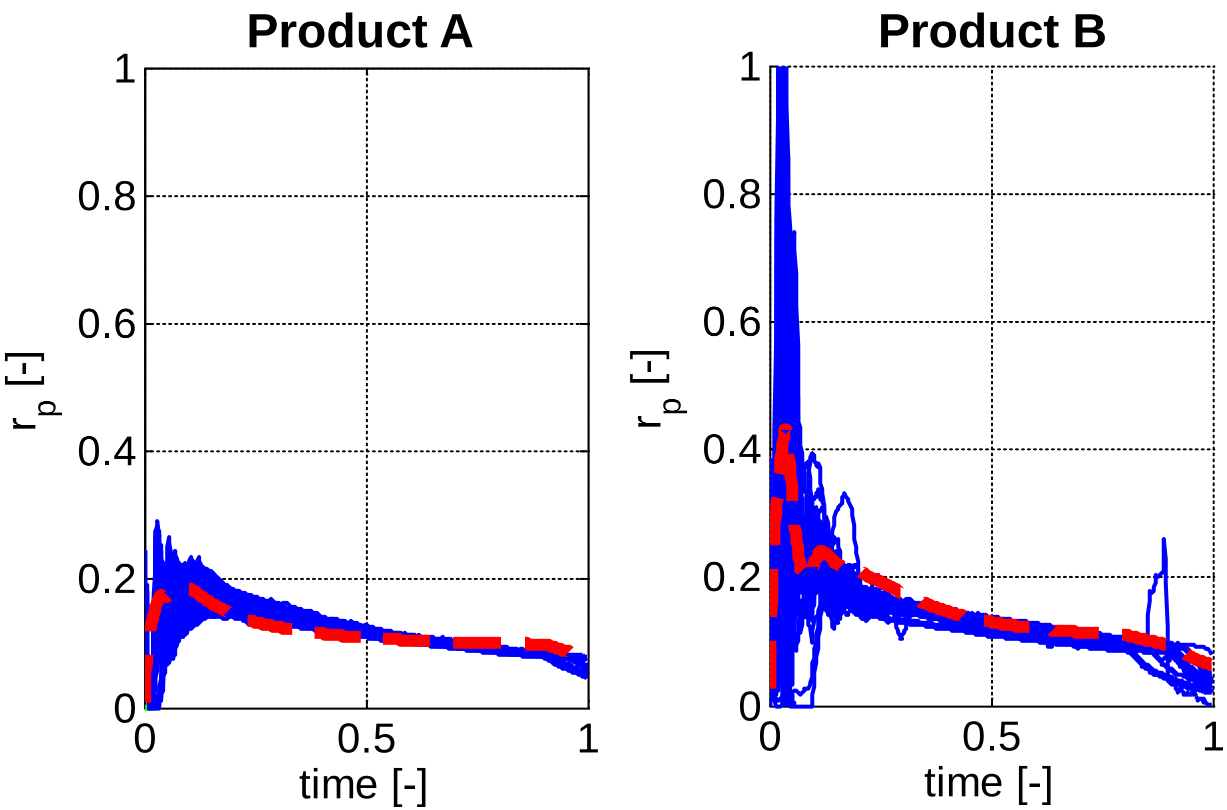
$$KA = C_1 M_R(t) - C_2 M_P(t)$$

Estimation of the reaction constants



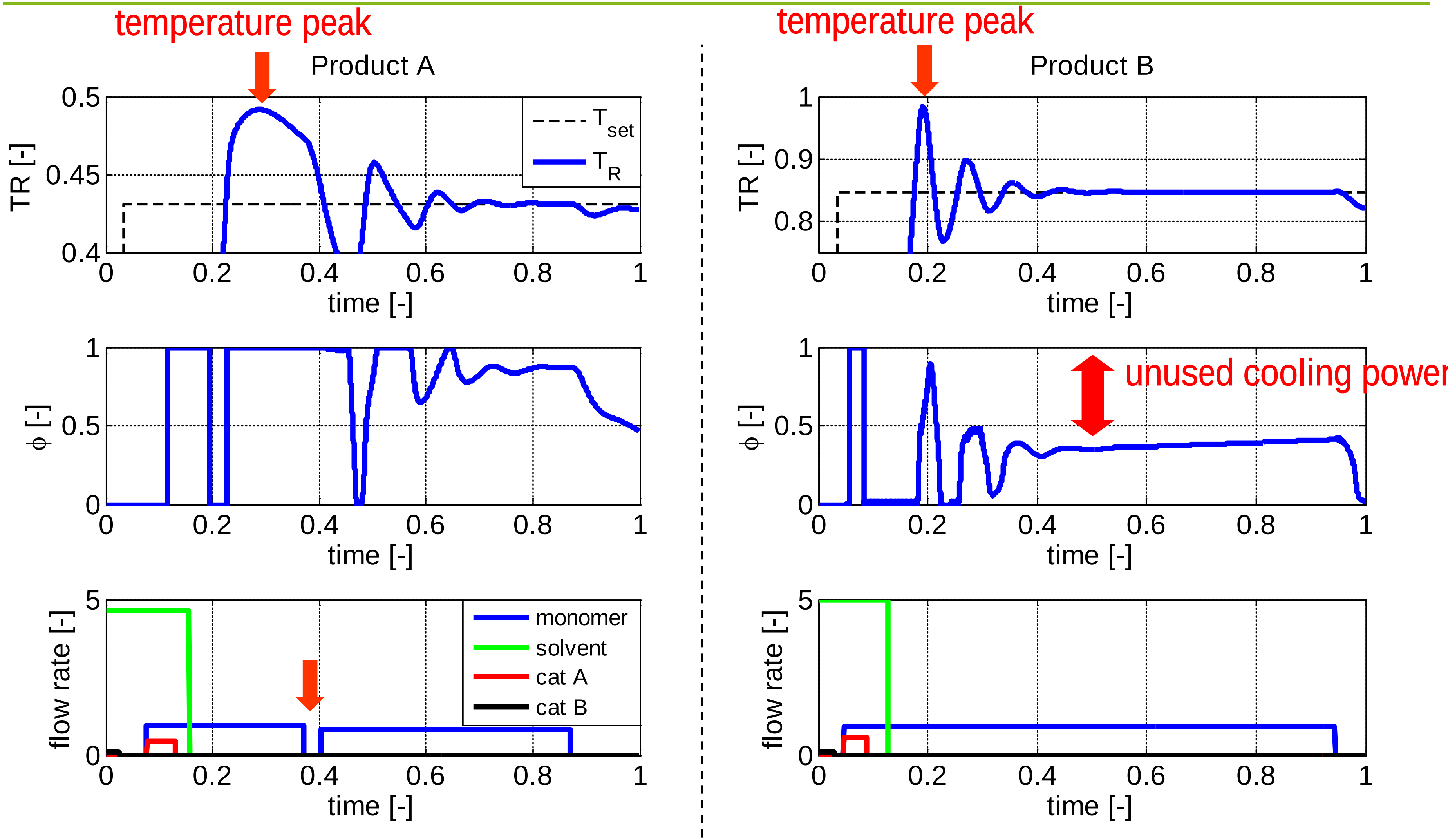
$$r_P = \frac{C_{P_R} M_R \frac{dT_R}{dt} - KA\left(T_J - T_R\right) - \sum_{i=S,M} F_i C_{P_i} \left(T_i - T_R\right)}{\Delta H_R}$$

Estimation of the reaction rate constants

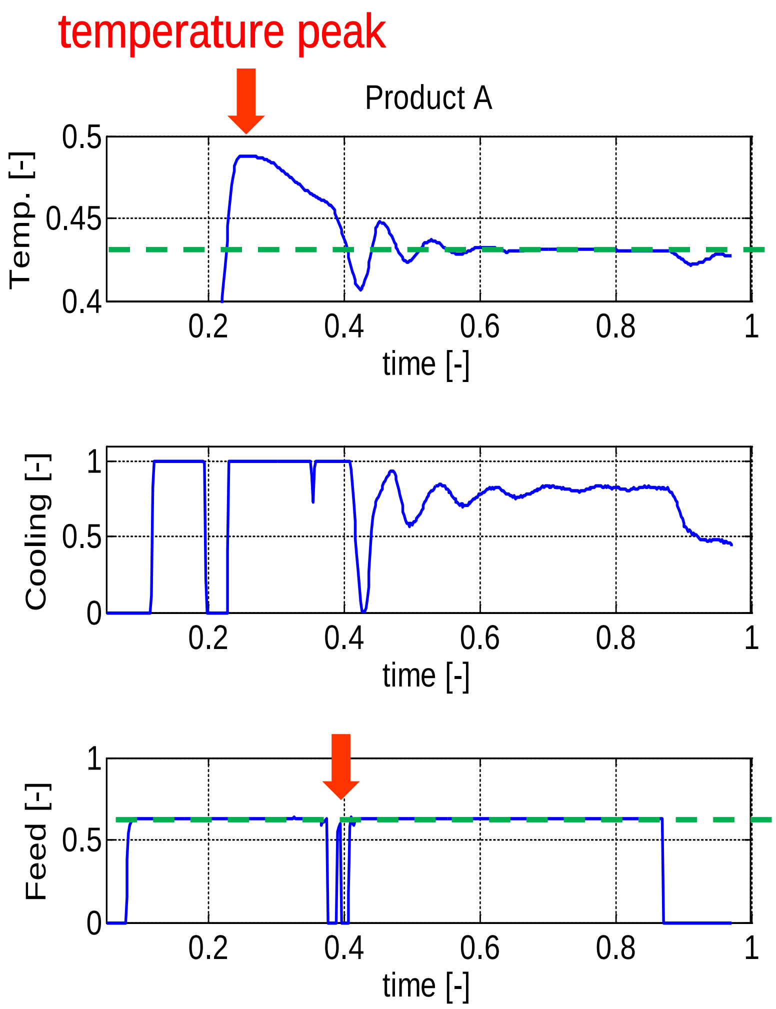


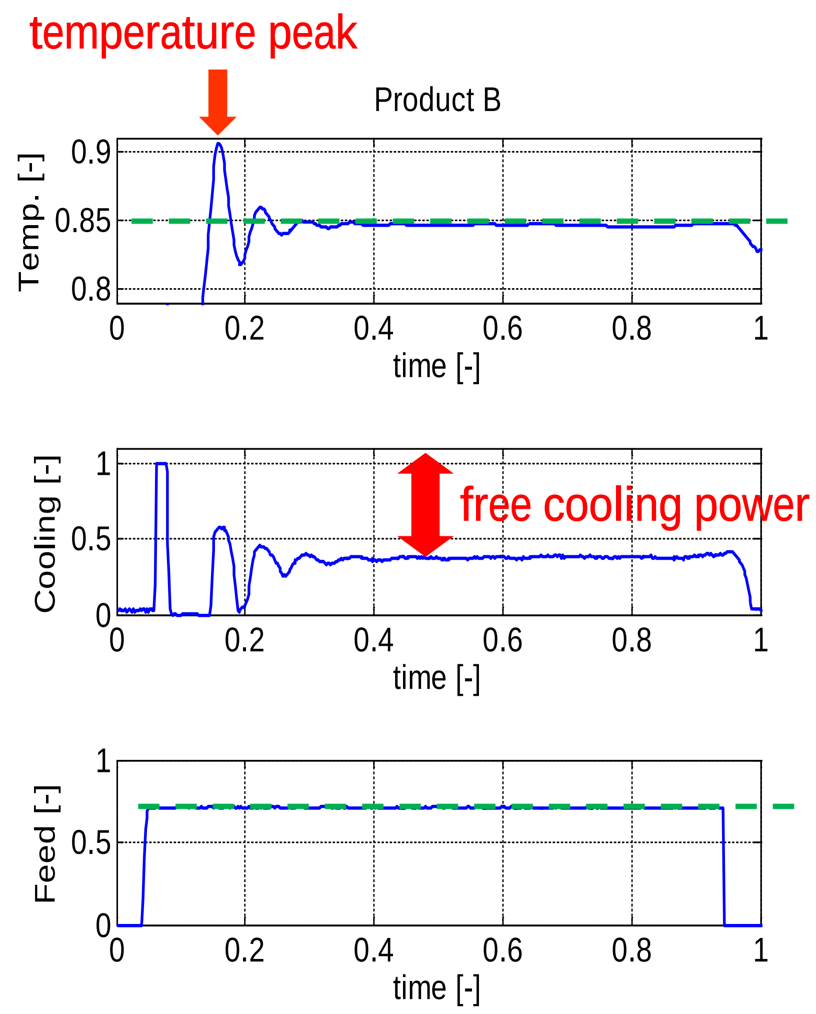
$$r_p = k_1 \exp\left(\frac{-Ea_1}{RT_R}\right) C_{P^*_{1,r}} C_M + k_2 \exp\left(\frac{-Ea_2}{RT_R}\right) C_{P^*_{2,r}} C_M$$

Closed-loop simulations



Real batch runs





Next step: Control solution

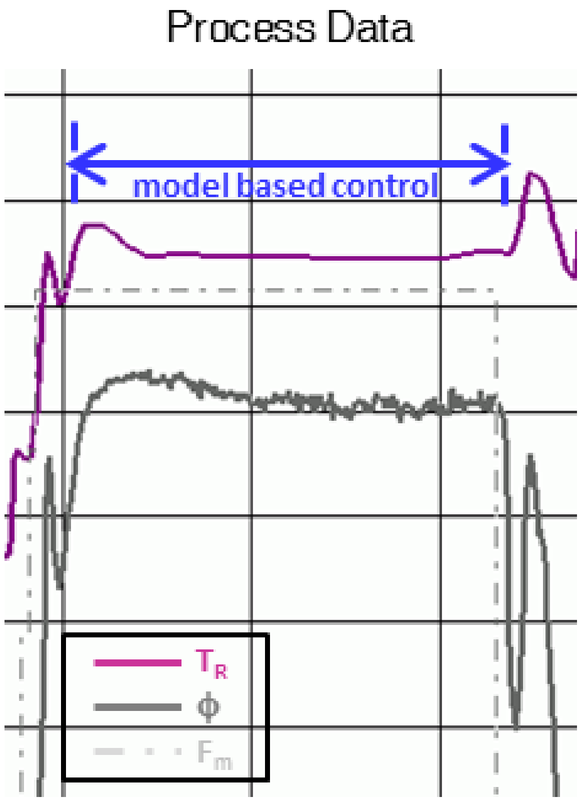
- So now we have a model – but of course the model is not exact
- Should we build a model-based controller upon it?
- How to take uncertainties into account?

- Solution 1:
  - MPC controller of the temperature (model-based, identified model)
  - Simple optimizing monomer flow controller

- Solution 2:
  - Model-based optimizing control using state and parameter estimation

Improved temperature control

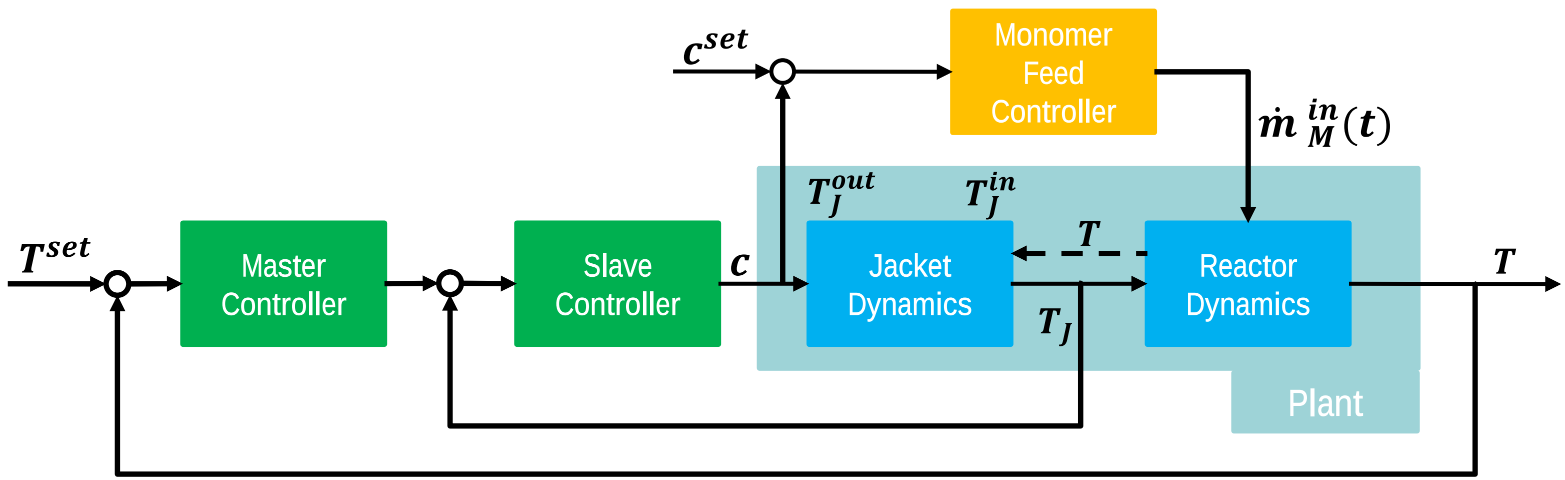
- A version of MPC of the temperature was integrated into the DCS of the real process
- The temperature peak was reduced to less than 0.5 K.
- The controller is used to control the temperature of the industrial reactor.



Near optimal operation by simple feedback control

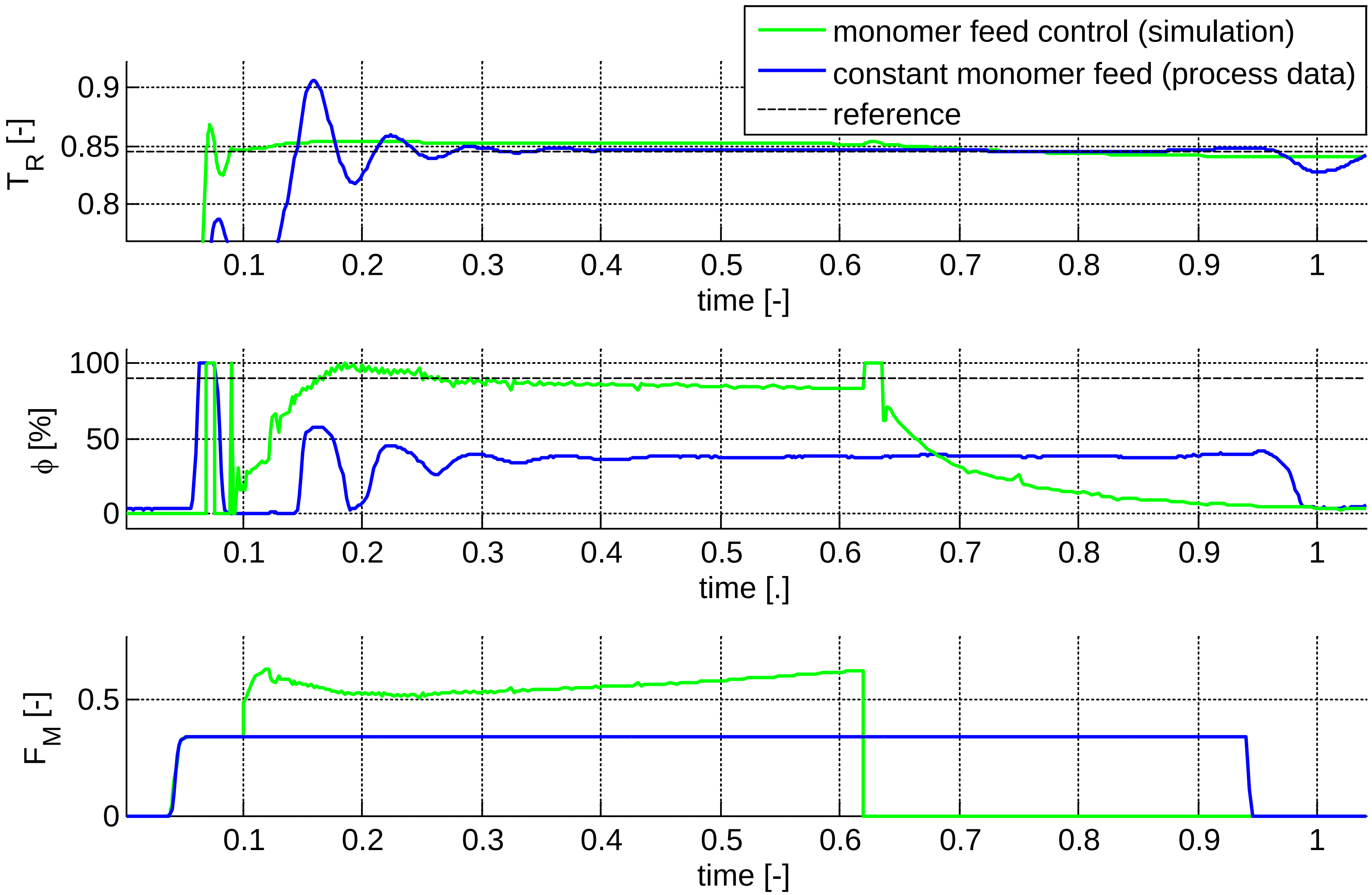
- Idea:

  Instead of online optimization, use a feedback controller that establishes an optimal operation (NCO tracking)
- Here: Make **full use of the available cooling power**



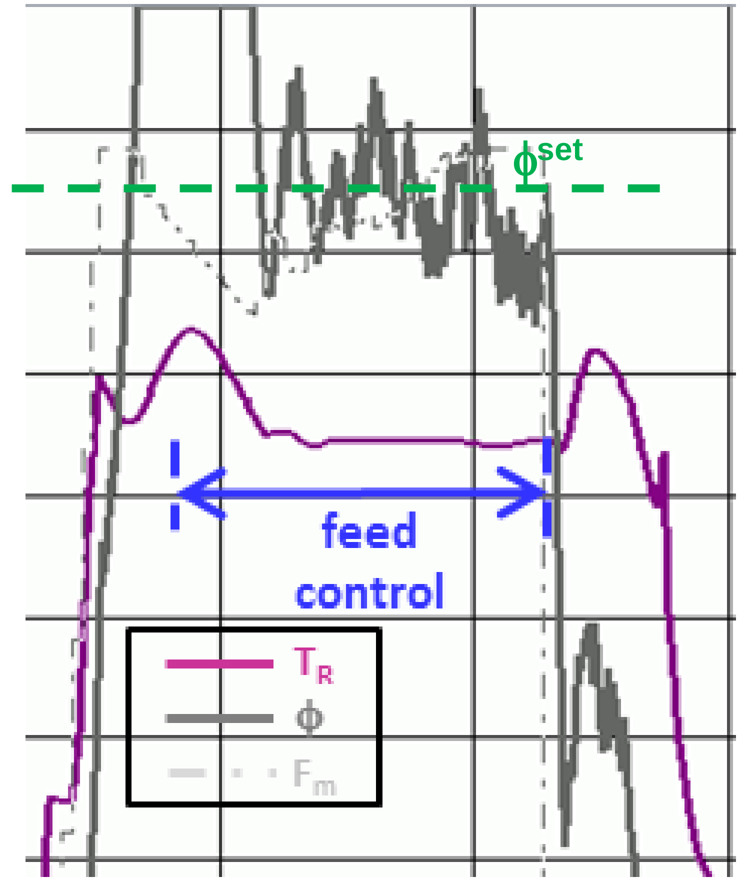
- Parameter c^{set} determines the spare cooling power

Monomer feed control simulated for the industrial case



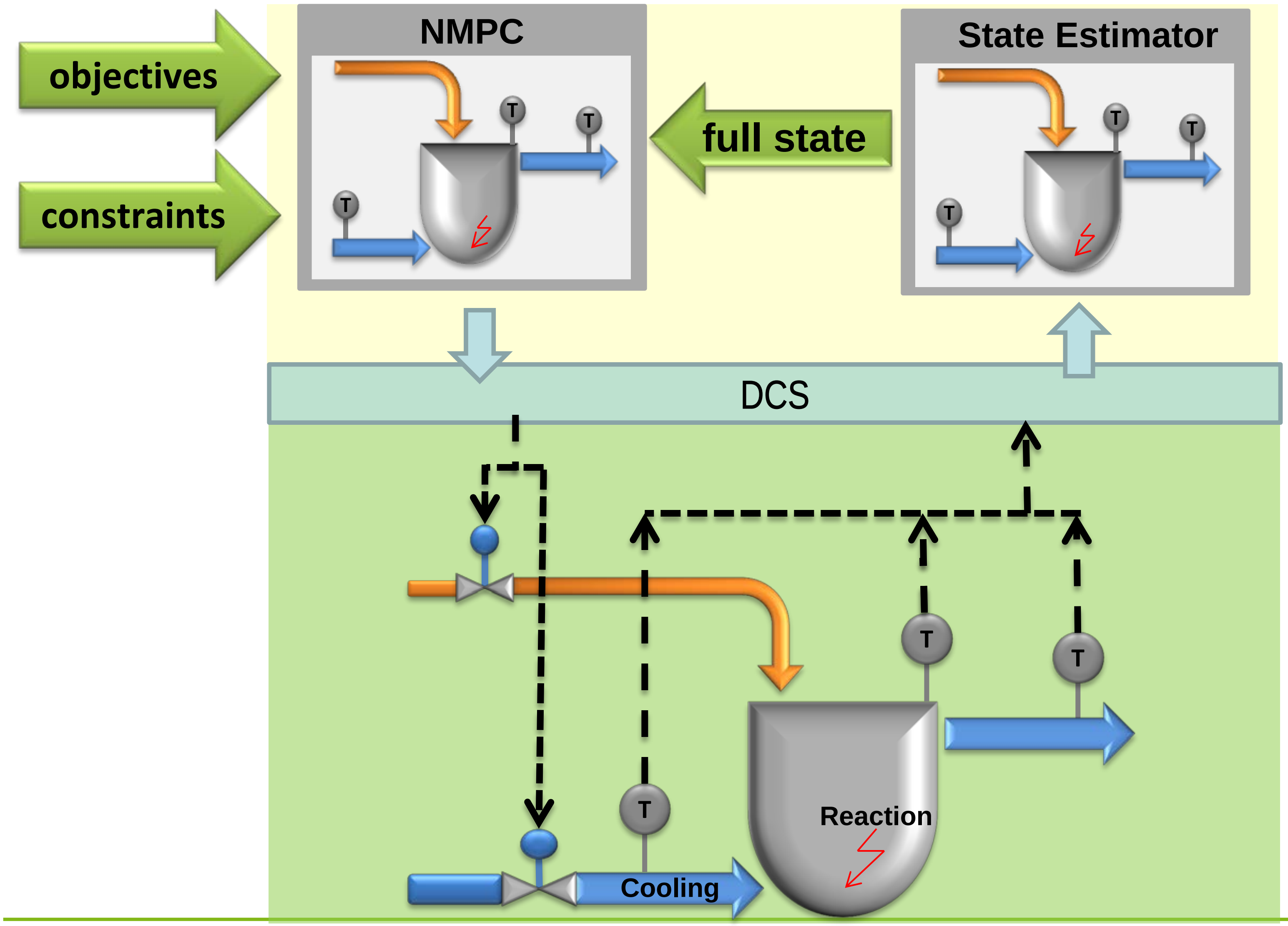
Implementation results

- Feedback controller for the monomer feed implemented at the plant
- Easy to realize in the DCS
- Successful stable operation
- Better temperature control thanks to the MPC controller and 25% reduction of the feeding times achieved
- Accepted by the operating crew
- In daily operation!!

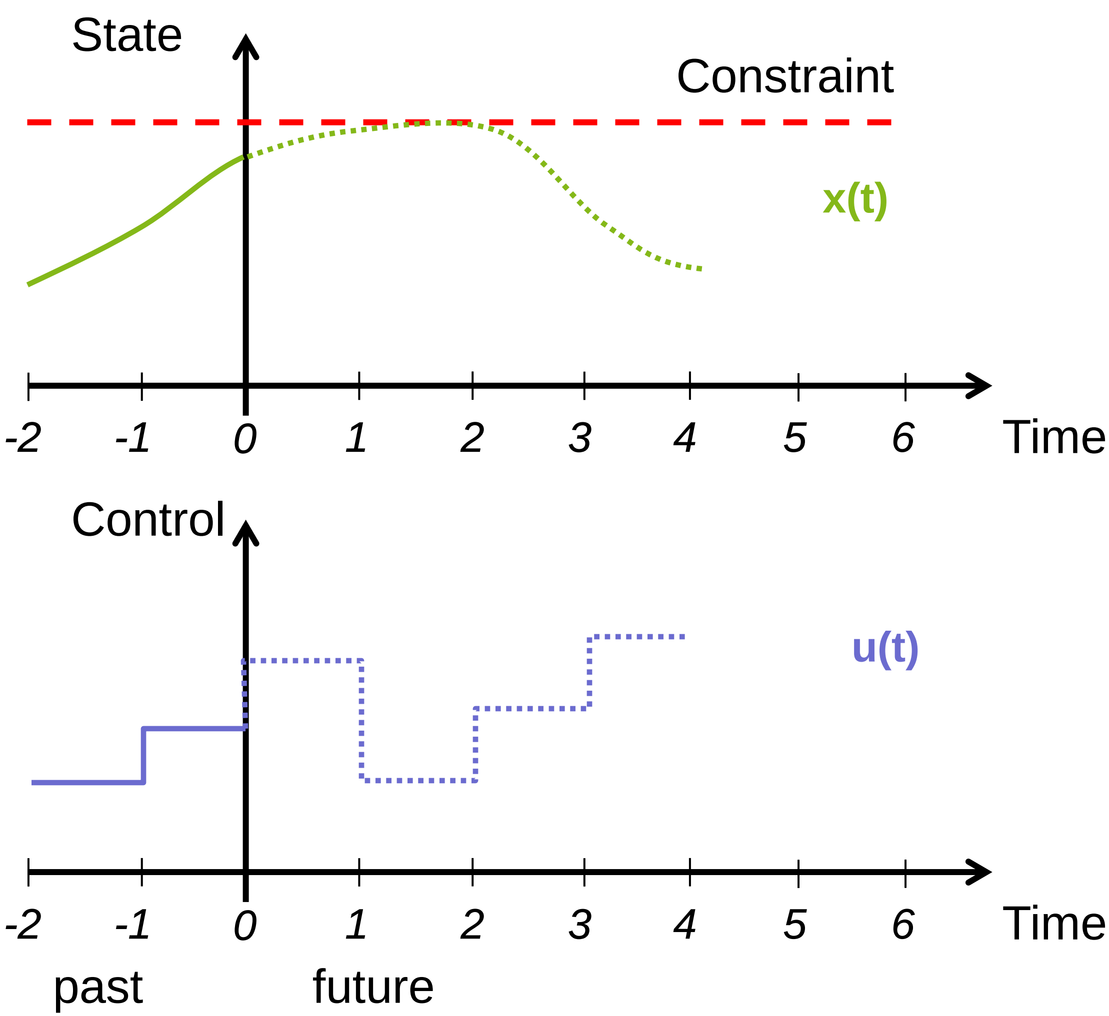


Process Data

Model-based control scheme



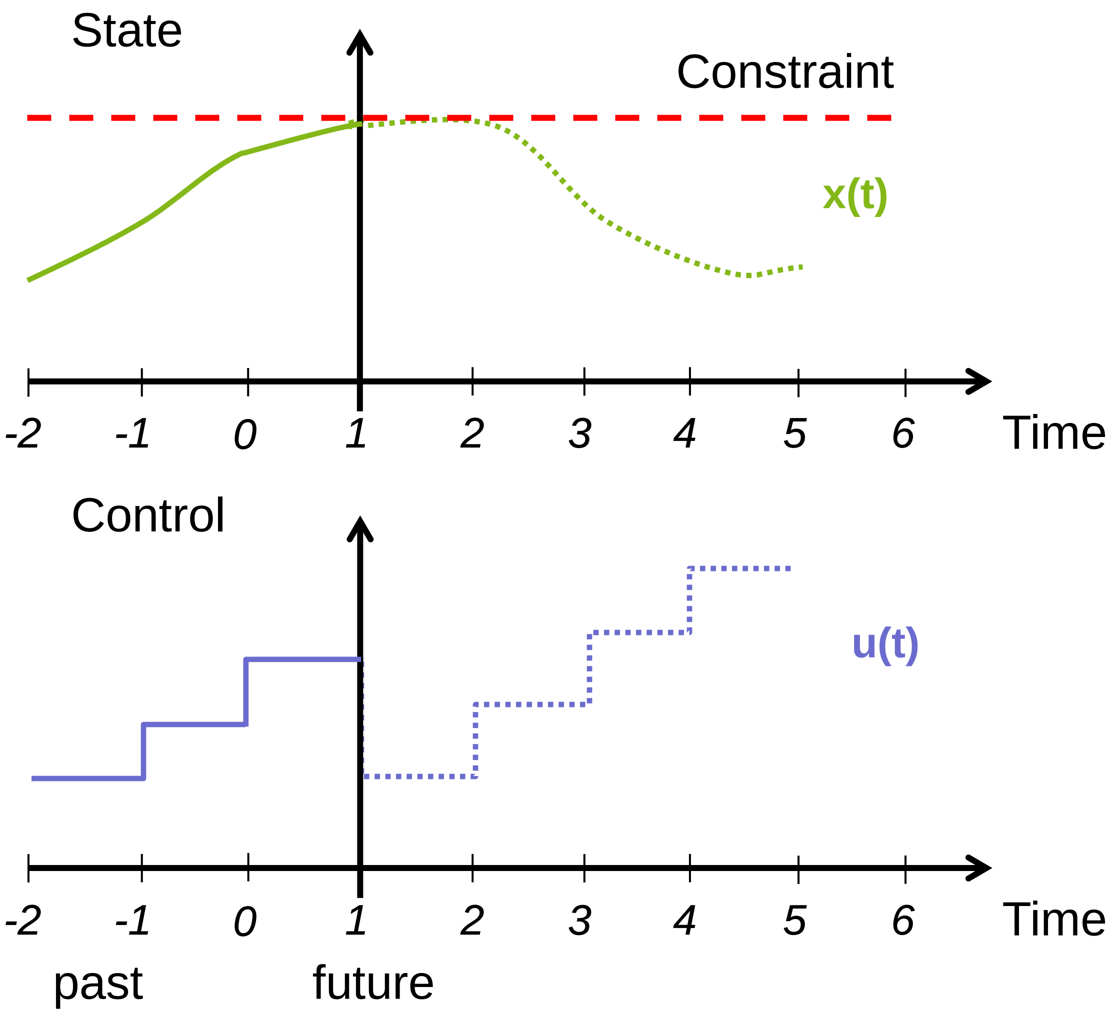
Model predictive control



MPC

- Solve optimization problem
  - Mathematical Model
  - Cost function
  - Constraints
- Apply first control input

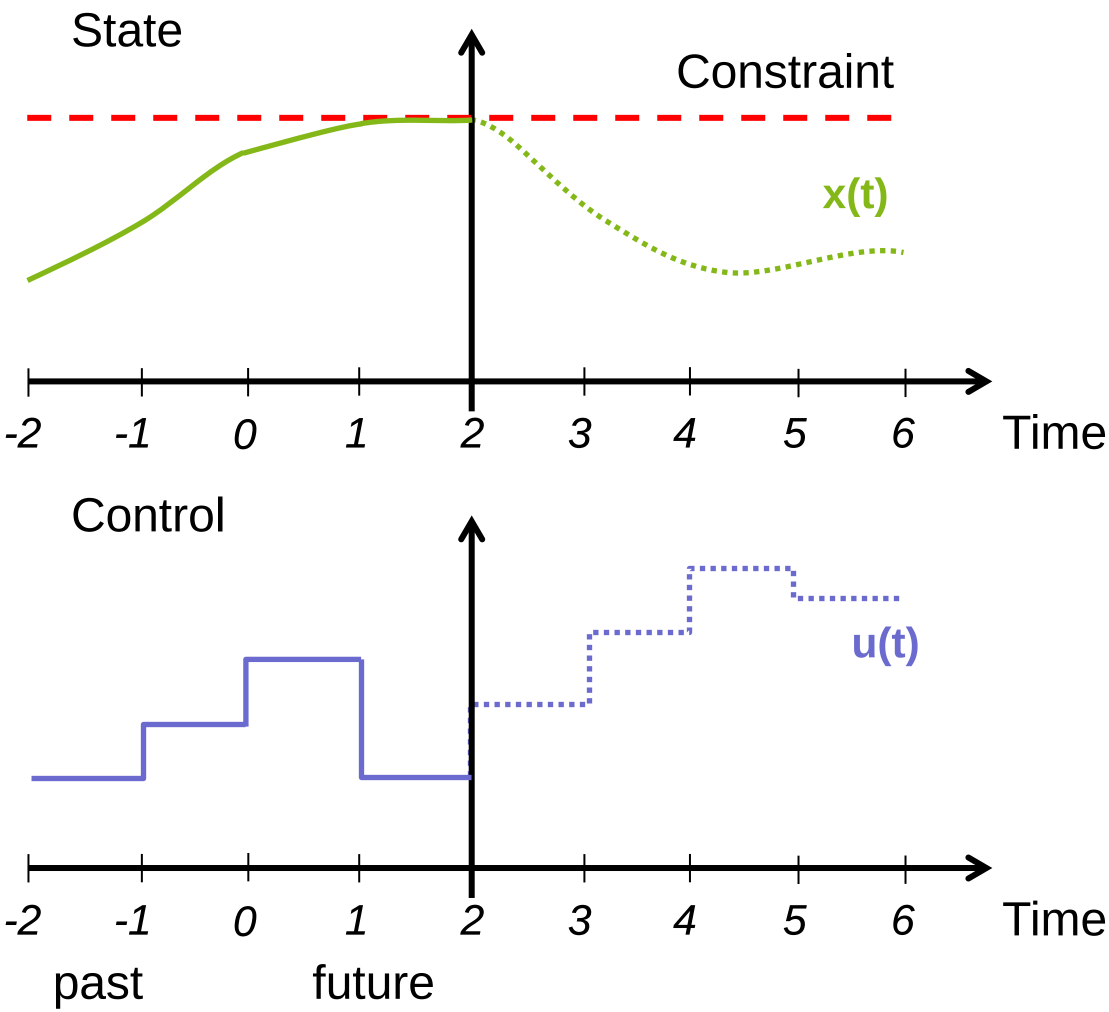
Model predictive control



MPC

- Solve optimization problem
  - Mathematical Model
  - Cost function
  - Constraints
- Apply first control input
- Take new measurements
- Optimize again

Model predictive control

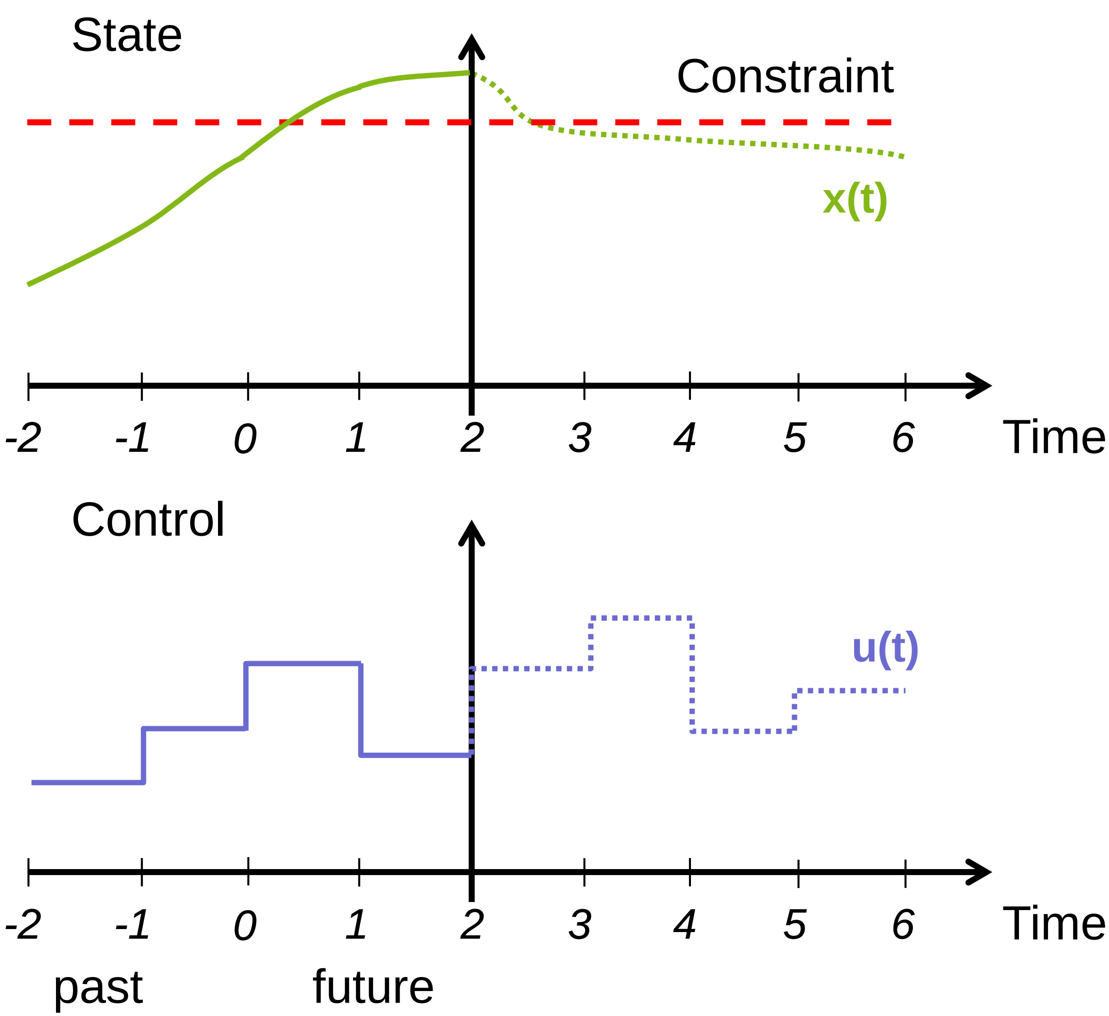


MPC

- Solve optimization problem
  - Mathematical Model
  - Cost function
  - Constraints
- Apply first control input
- Take new measurements
- Optimize again
- Apply first control input
- Take new measurements and optimize again ….

- Economic cost function can be used in the optimization
  → **optimizing control**

Model Predictive Control: Wrong model



MPC

- Solve optimization problem
  - Mathematical Model
  - Cost function
  - Constraints
- Apply first control input
- Take new measurements

What happens if the prediction is not exact?

- Violation of constraints
- Decreased performance
- Instability

Industrial example – online model adaptation

- Reduced model
  - 6 mass balances, 3 energy balances, 6 moment balances
- Simplified kinetics:

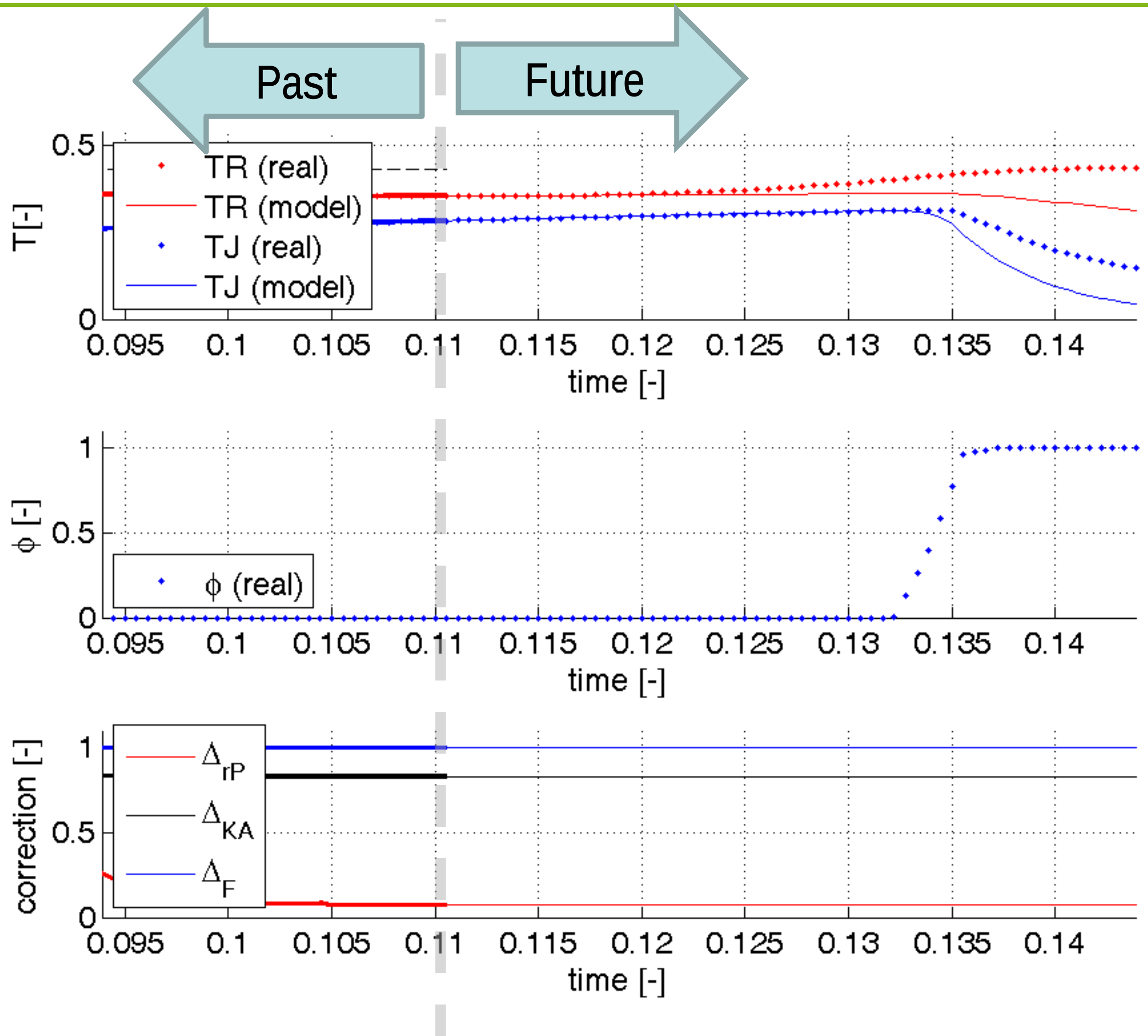
$$\left.\begin{array}{l} CAT_A + M + CAT_B \xrightarrow{k_i} C^* \\ M \xrightarrow{C^*} P \end{array}\right\} \qquad r_p = k_p \exp\left(\frac{Ea}{RT_R}\right) C_{C^*} C_M V$$

- Online compensation of uncertainties:

$$\begin{cases} r_p^* = \left(k_p \exp\left(\frac{Ea}{RT_R}\right) C_{C^*} C_M V\right) \Delta_{r_p} \\ KA^* = \left(C_1 M_R(t) - C_2 M_P(t)\right) \Delta_{KA} \\ F_{cool}^* = \left(\beta_1 \phi + \beta_2 \phi^2 + \beta_3 \phi^3 + \beta_4 \phi^4\right) \Delta_{F_{cool}} \end{cases}$$

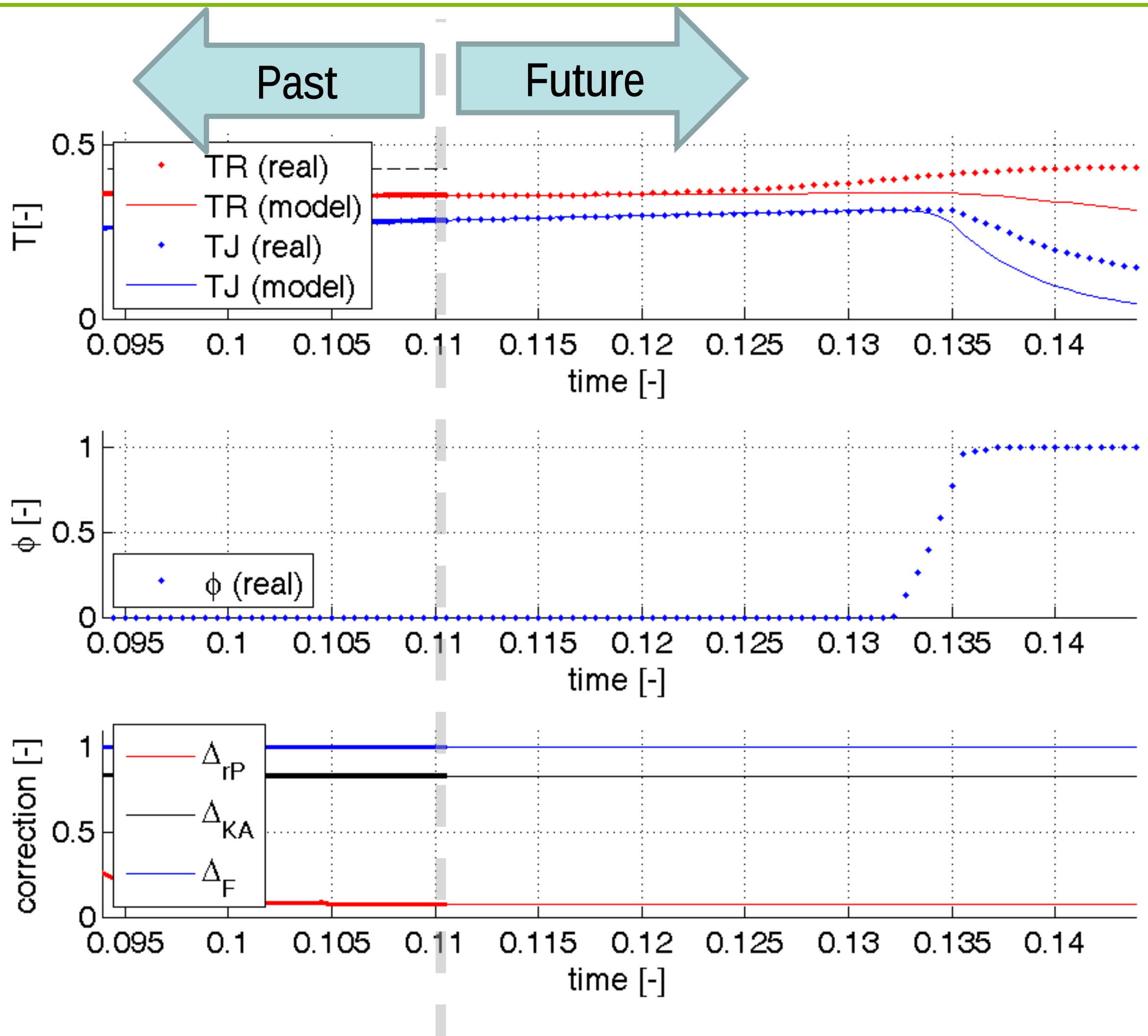
Correction factors are estimated by the state estimator.

Testing for real batch data



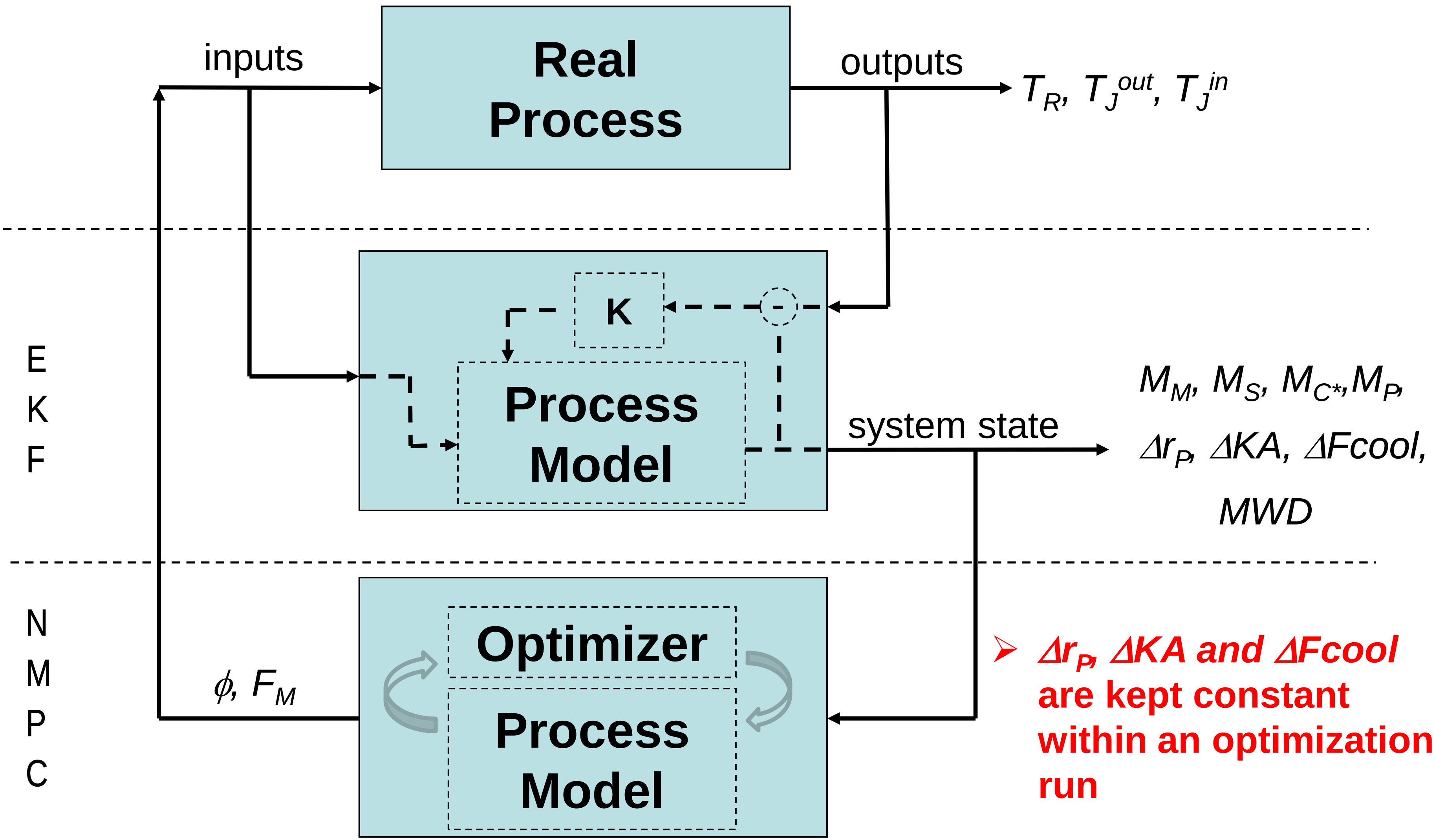
- Measurements taken from a real batch (dots)
- The measurements are fed to the EKF and the correctors are updated.
- The model is repeatedly simulated from the current time point (continuous lines)
- The correctors are kept constant during each simulation.

Testing for real batch data



- Measurements taken from a real batch (dots)
- The measurements are fed to the EKF and the correctors are updated.
- The model is repeatedly simulated from the current time point (continuous lines).
- The correctors are kept constant during each simulation.

Block diagram of the closed-loop



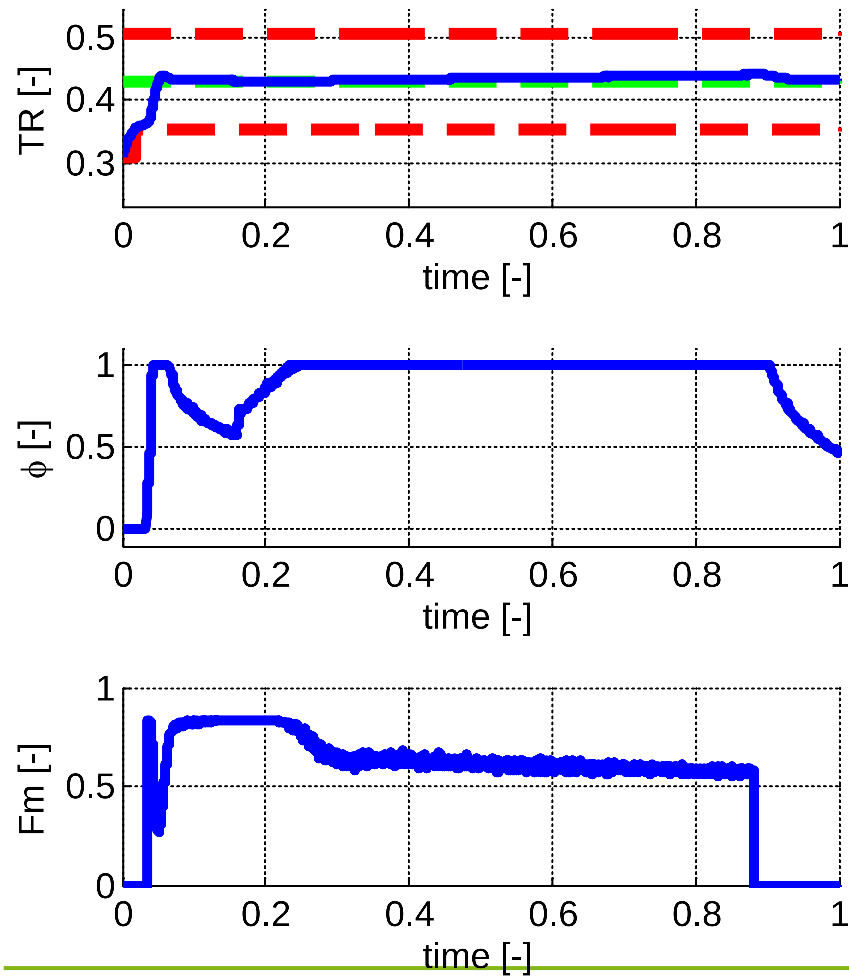
- **Δr_P, ΔKA and $\Delta Fcool$ are kept constant within an optimization run**

NMPC simulation

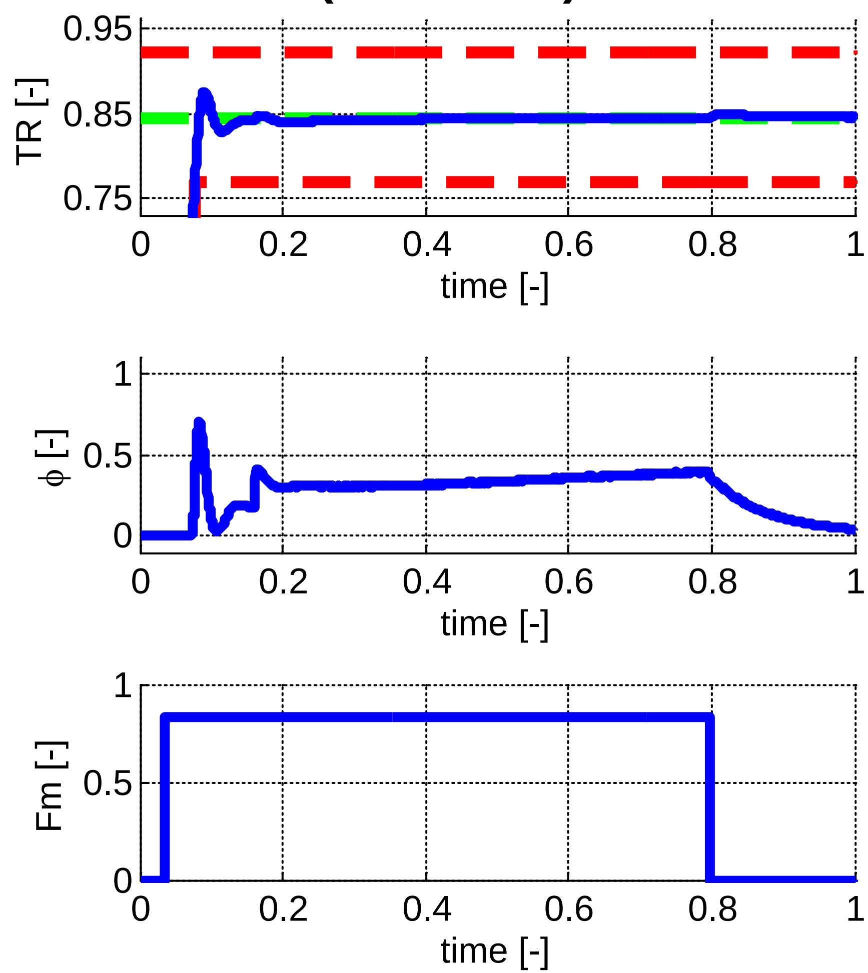
- NMPC setup was intensively tested by simulations
- Controller Settings:
  - Prediction horizon: 10 minutes
  - Control horizon: 10 minutes
  - Discretization period: 2 minutes
  - Sampling period: 10 seconds
- Plant-model mismatches:
  - reaction rate: $\pm$50%
  - heat transfer efficiency: $\pm$ 25%
  - cooling capacity: $\pm$50%

Simulation (Normal reactivity)

Automatic Monomer Feed (Product A)

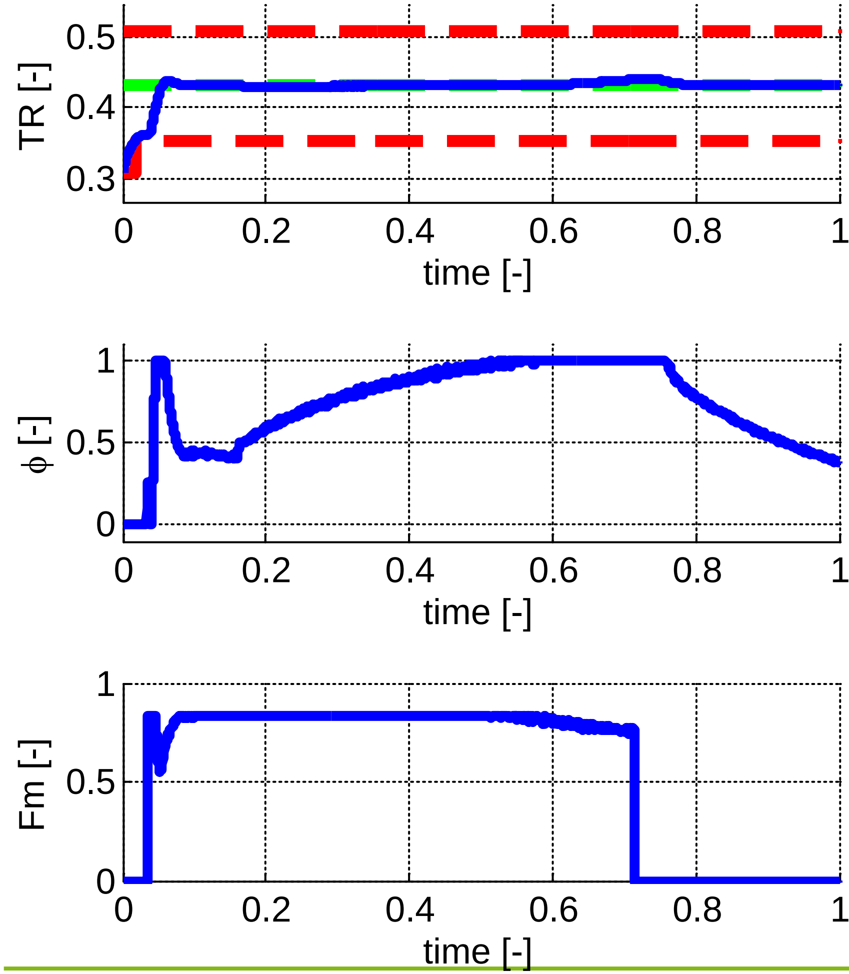


Constant Monomer Feed (Product B)

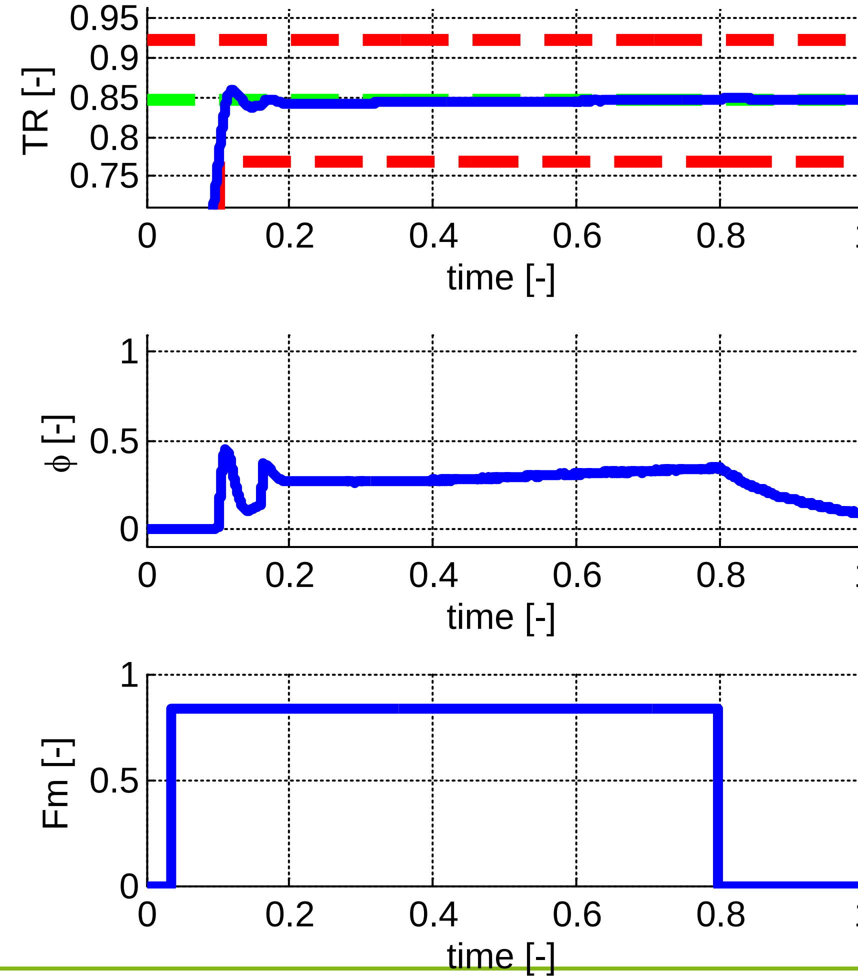


Simulation (Low reactivity)

Automatic Monomer Feed (Product A)

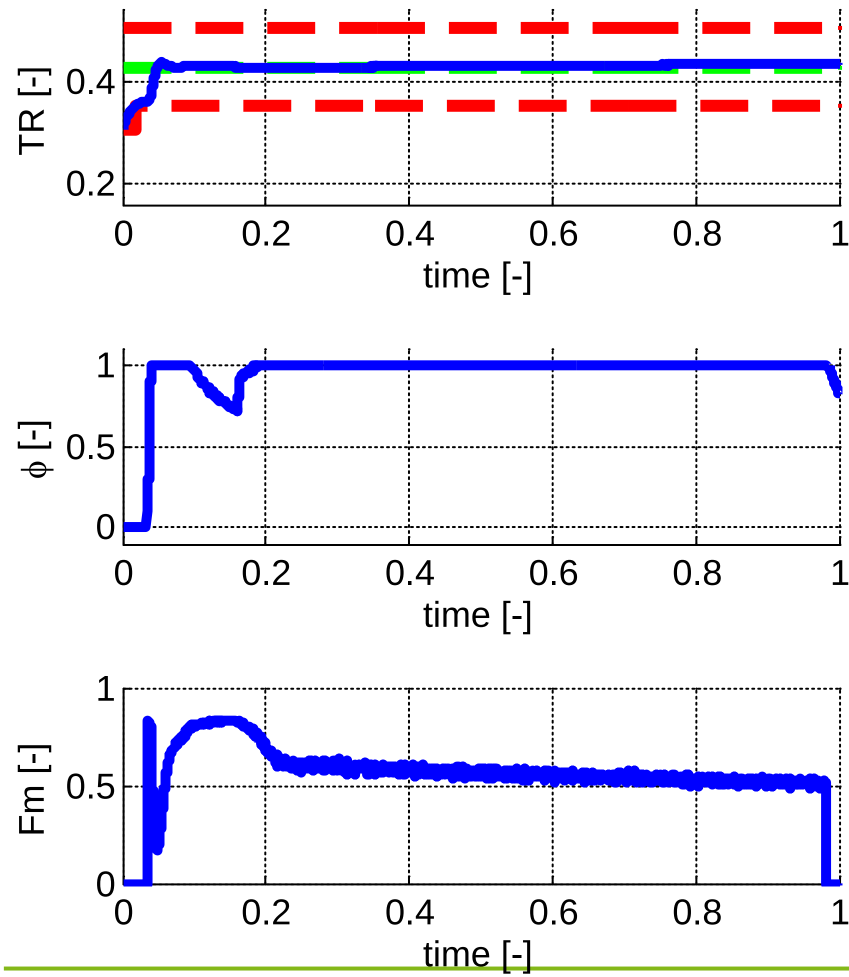


Constant Monomer Feed (Product B)

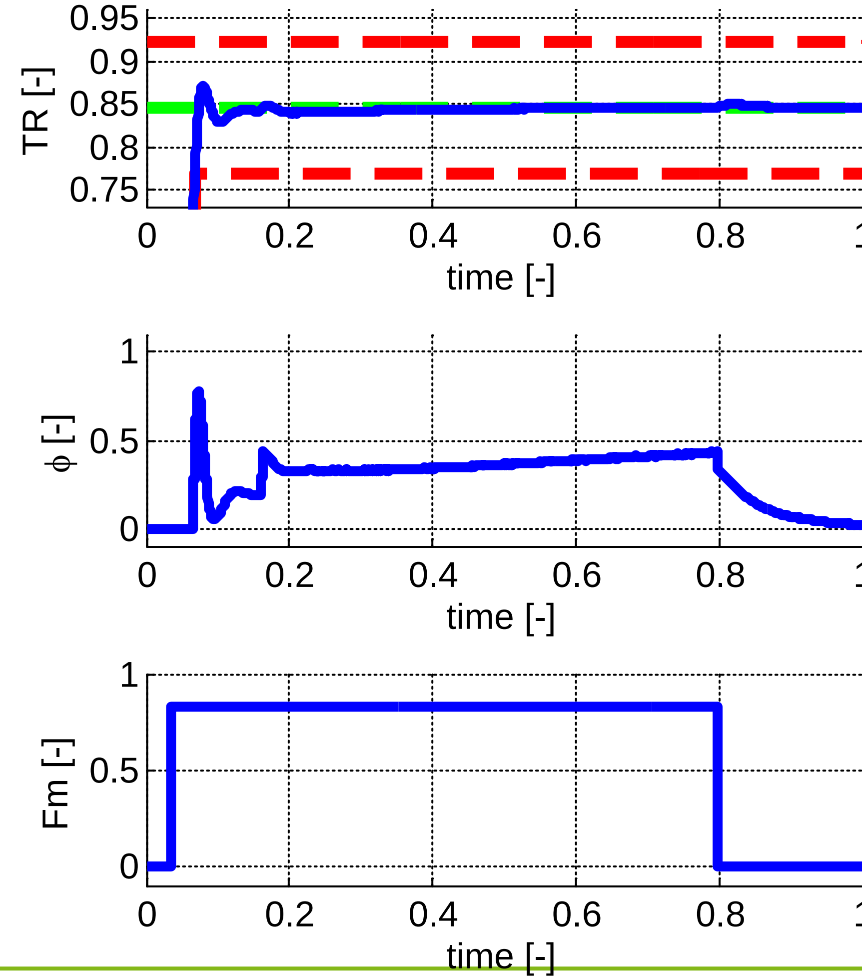


Simulation (High reactivity)

Automatic Monomer Feed (Product A)



Constant Monomer Feed (Product B)

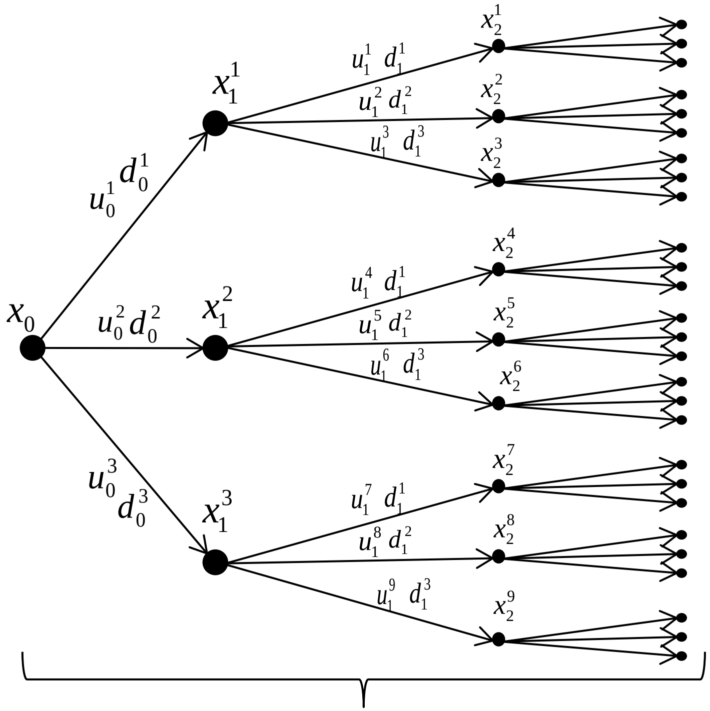


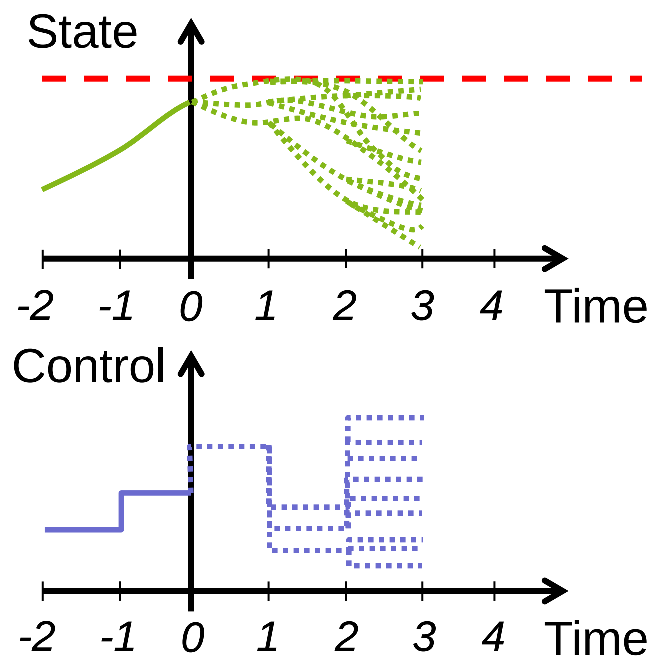
Conclusions

- Combined state and parameter estimation is feasible
  - Constraint: At least as many independent measurements as unknown parameters are needed!

- How can the robustness of the controller be improved or even guaranteed?

Multi-stage NMPC: Formulation

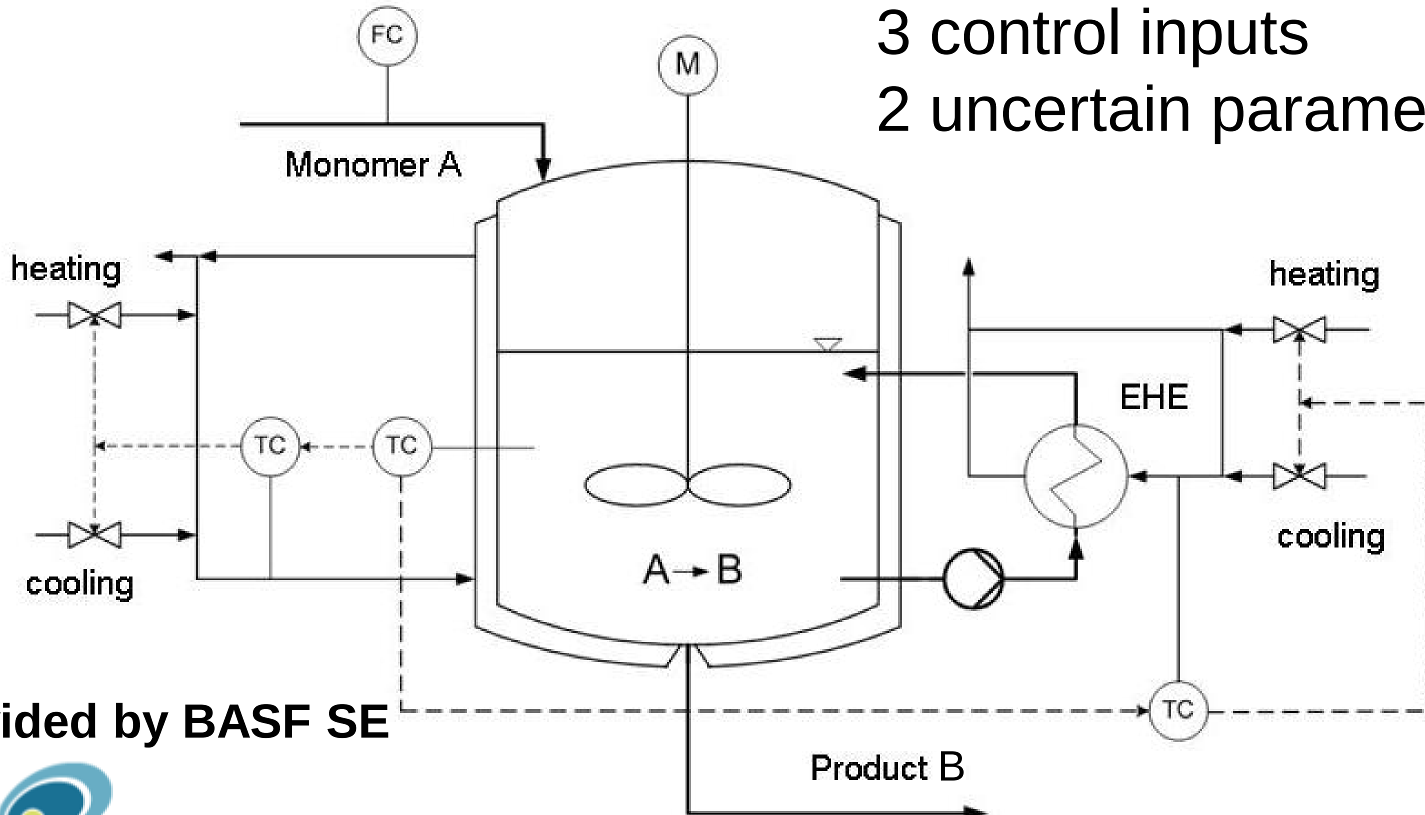




- Uncertainty is modelled by a scenario tree
- Constraints must be met for all values of the uncertainty
- Controller will react to the information gained at the next stage
- This is taken into account in the optimization of the next decisions

An industrial batch polymerization reactor control problem

8 differential states
3 control inputs
2 uncertain parameters



Model provided by BASF SE

EMBOCON

[Lucia, Andersson, Brandt, Diehl & Engell, JPC, 2014]

Formulation of the NMPC problem

- Control task:
  - Minimize the batch time while satisfying temperature constraints for all the values of two uncertain (±30 %) parameters

- Standard NMPC with tracking cost:

$$J_{\text{track}} = \sum_{k=0}^{N_p-1} -m_{P,k}^{j} + q\left(T_{R,k}^{j} - T_{\text{set}}\right)^2 + r\, \Delta \mathrm{u}_{\mathrm{k}}^{\mathrm{j}\;2}$$

- Multi-stage NMPC with economic cost function:

$$J_{\text{eco}} = \sum_{i=1}^{N} \omega_i \sum_{k=0}^{N_p-1} -m_{P,k}^{j} + r\, \Delta \mathrm{u}_{\mathrm{k}}^{\mathrm{j}\;2}$$

Standard NMPC: No uncertainties

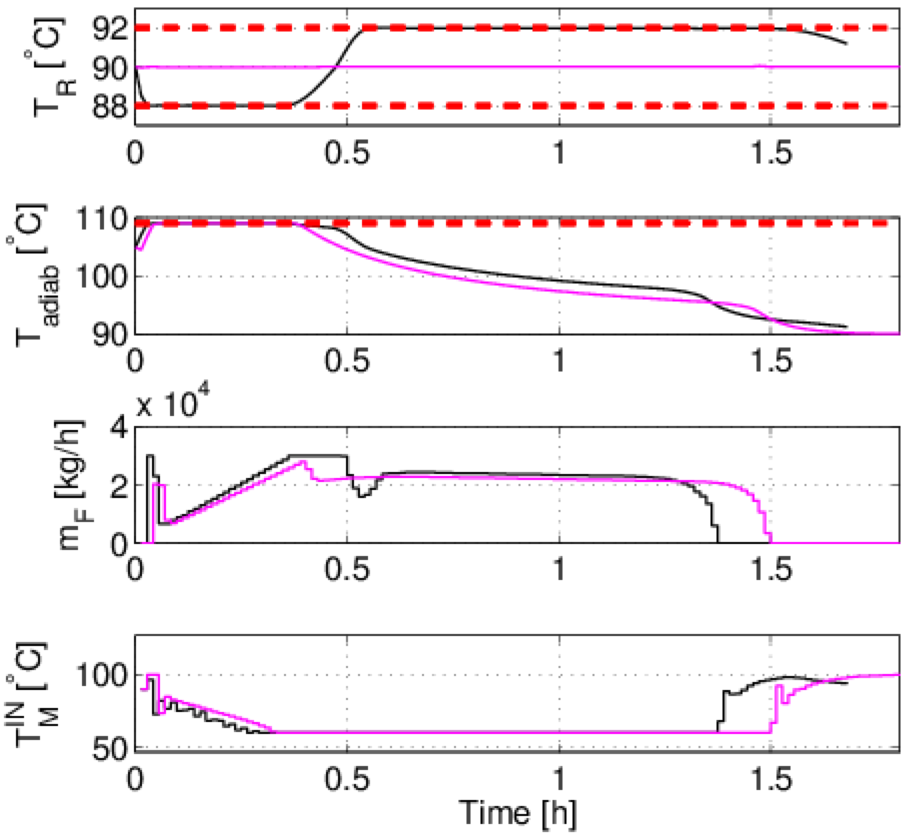
- Comparison of tracking and economic NMPC

Reactor temperature

Adiabatic temperature

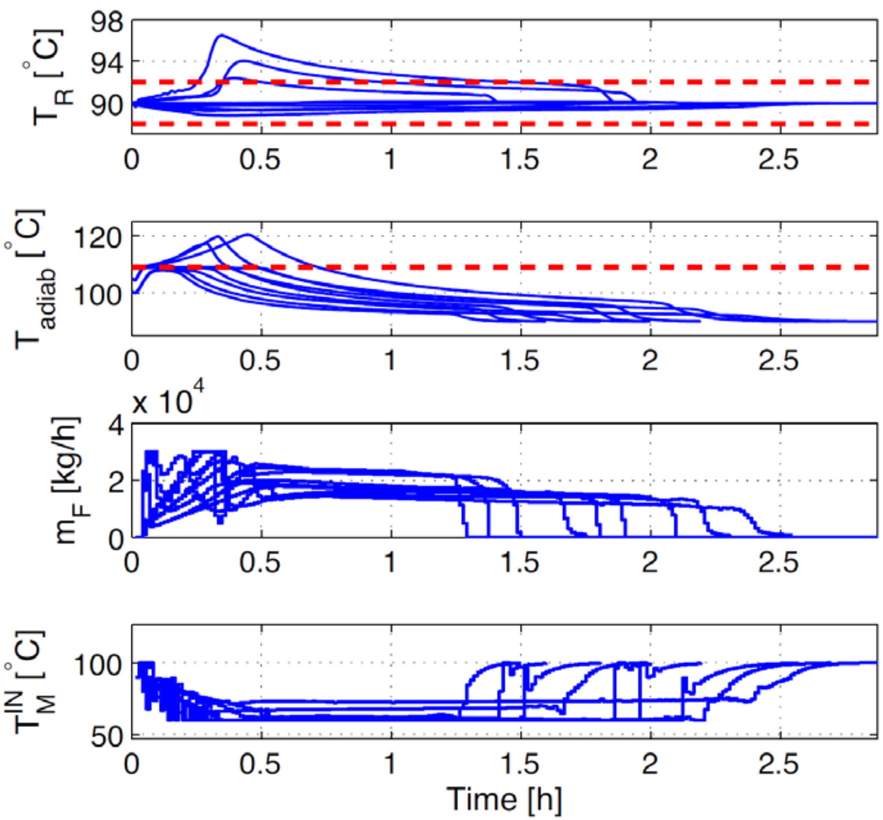
Monomer feed rate

Jacket inlet temperature

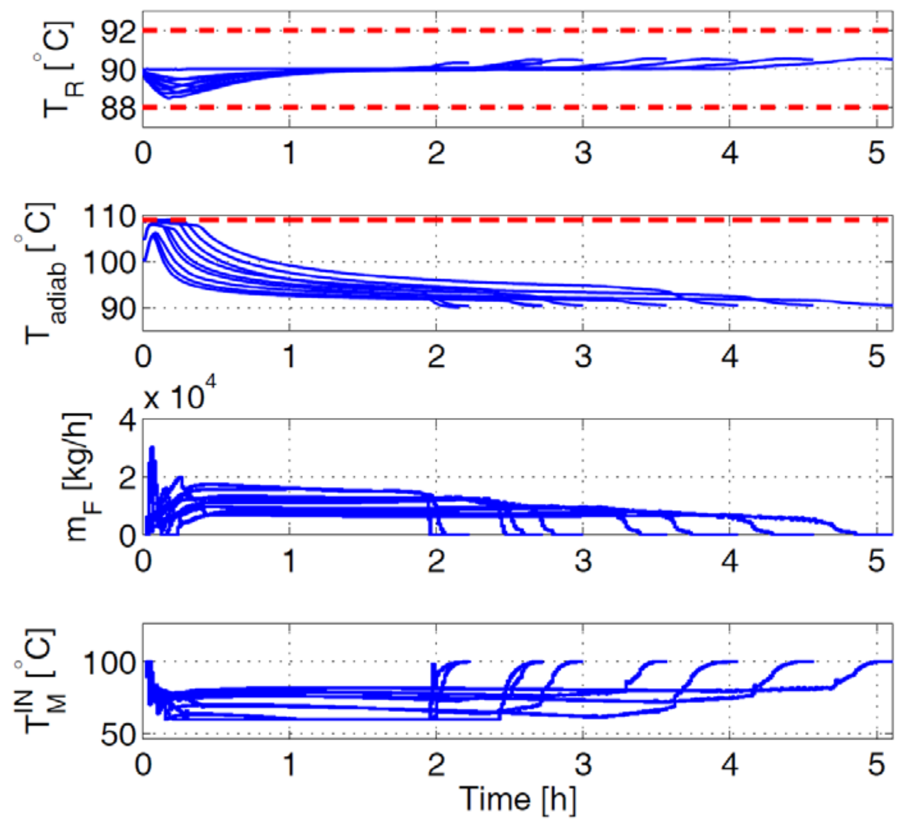


Simulation results for different scenarios

Standard NMPC



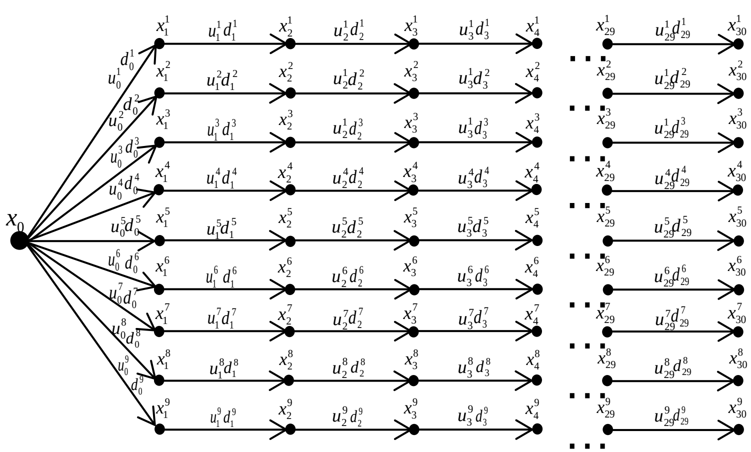
Standard NMPC with conservative choice of parameters



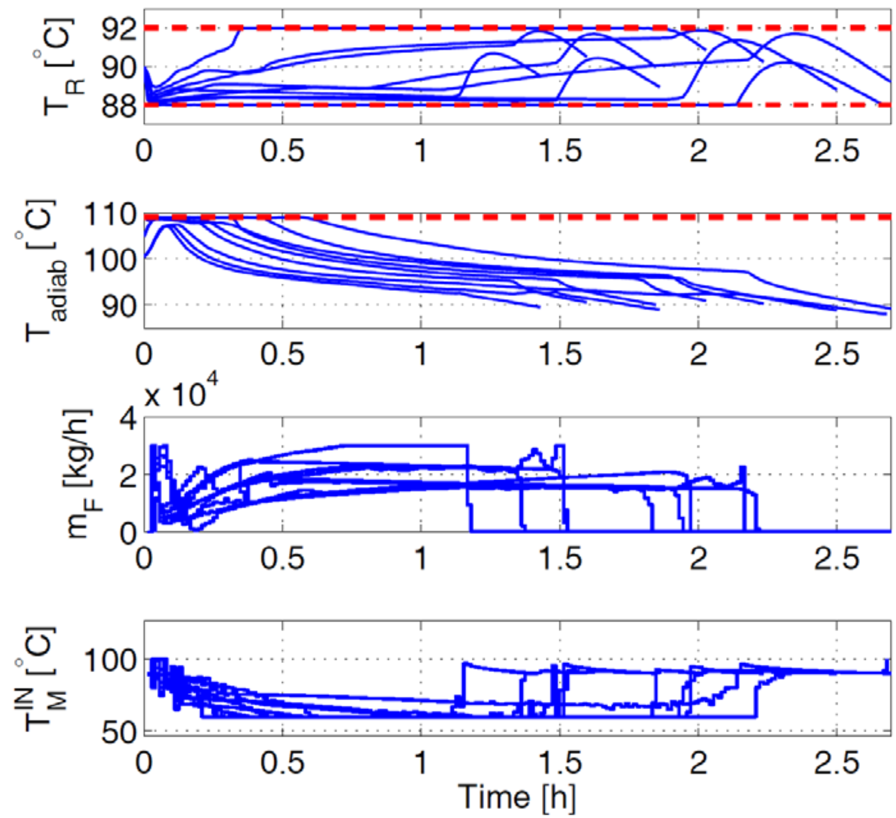
Simulations for different values of k and ΔH $(\pm 30\%)$

Simulation results for different scenarios

- Simple scenario tree
  - Extreme values of the uncertainty
  - Branch the tree only one stage



Multi-stage NMPC



Simulations for different values of k and ΔH ($\pm 30\%$)

Comparison with standard NMPC

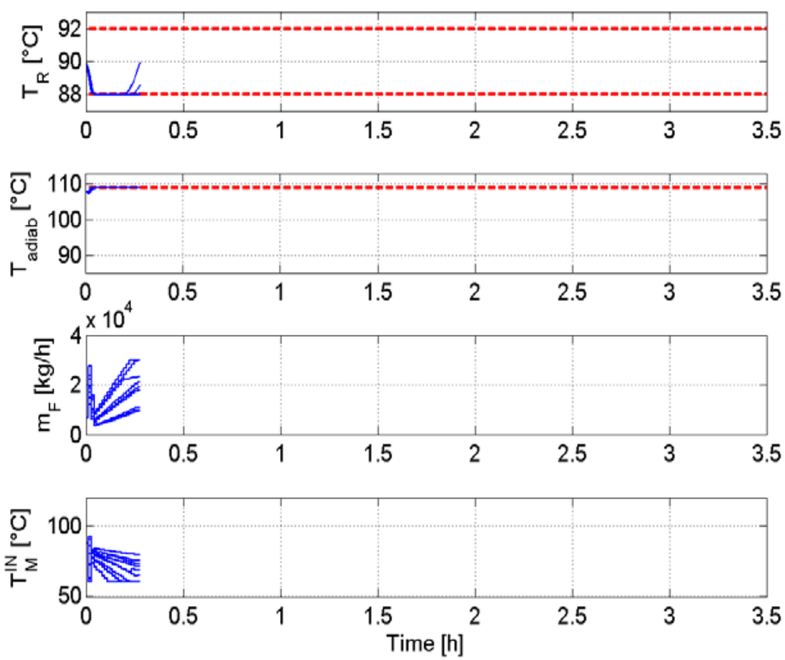
Scenario		Batch time in hours		
ΔH_R	k_0	Standard NMPC	Standard (cons.)	Multi-stage
+30%	+30%	infeasible	2.15	2.03
+30%	0%	infeasible	2.72	2.24
+30%	-30%	infeasible	4.05	2.69
0%	+30%	1.60	2.22	1.60
0%	0%	1.81	3.00	1.84
0%	-30%	2.69	4.57	2.50
-30%	+30%	1.50	2.72	1.43
-30%	0%	1.99	3.57	1.86
-30%	-30%	2.88	5.11	2.68
Av. batch time [h]		infeasible	3.35	2.10

- Batch time reduction of 60% w.r.t. standard (cons.) NMPC

Comp time [s]	Standard NMPC	Standard (cons.)	Multi-stage
Average	0.072	0.059	1.134
Maximum	0.230	0.179	1.550

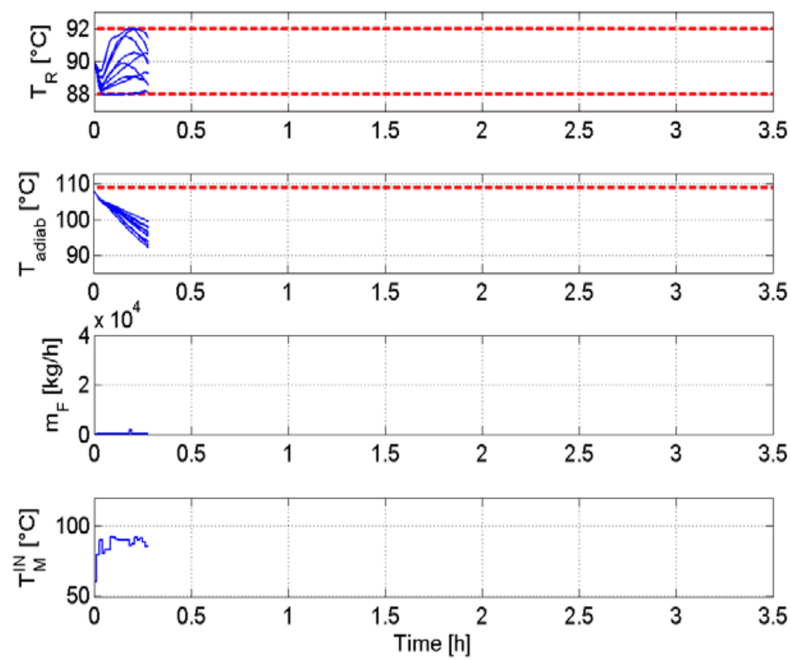
Comparison with open-loop robust NMPC

Multi-stage NMPC



Open-loop robust NMPC

~ 25% longer batch!



Multi-stage optimizing control - conclusions

- The improvement of the robustness is very convincing.
- Direct solution without a need for specific engineering
- Improvement over nominal NMPC even when parameter updates are available
- Numerically tractable

Summary

- Advanced control offers a significant potential for improved operations.
- **One can control well without an exact model!**
- Different solutions presented:
  - Tracking of optimality conditions – purely measurement based
  - Adaptation of a simplified prediction model
  - Multi-stage robust model-based optimization
- Modeling effort is the bottleneck in the solution of practical problems.
  - **Robust formulations reduce the modeling effort**
- **Unresolved problem**:
  Satisfaction of complex product property constraints
  - Direct measurements (e.g. Raman)
  - Soft sensors with additional online measurements - not necessarily selective, e.g. ultrasound, conductivity, pH, turbidity
  - But must be calibrated

Copolymerization – Simulation study

- Simulation study of a seeded semi-batch copolymerization
  - Industrial scale
  - Styrene and butyl acrylate
  - Seeded semi-batch process
  - Only temperature control
- Assuming a correct model that predicts the sound velocity
- Comparison of state estimator performances
  - Based on temperature measurements
  - Based on temperature and sound velocity measurements

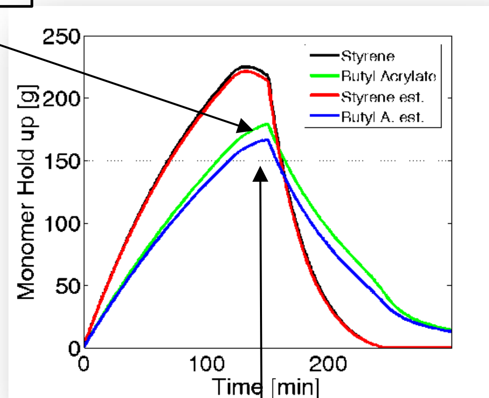
Copolymerization – Simulation Study

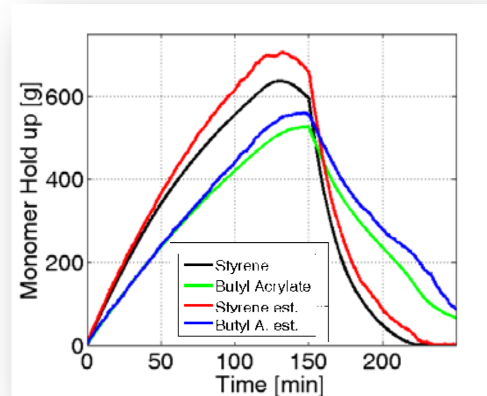
Mismatch in reactivity ratios (+/-10%)

kp_{11}-10%, kp_{22}+10%, $\Delta H_{R,1}$-10%, $\Delta H_{R,2}$+10%

Maximum offset 6.5%

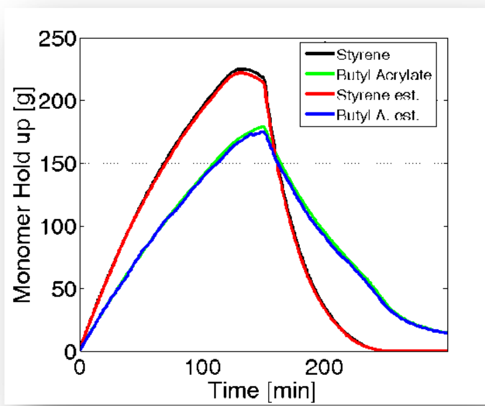
State estimator based on temperature

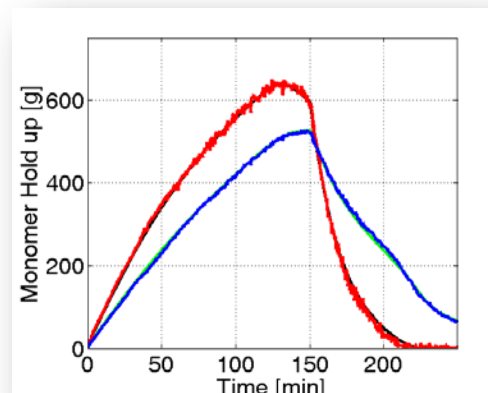




Feed stop

State estimator based on temperature and sound velocity





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- Land NRW (CheK NRW)
- ERC Advanced Investigator Grant MOCOCON

THANK YOU VERY MUCH FOR YOUR KIND ATTENTION!