Real-Time Optimization in the Presence of Uncertainty

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Process Control'11
Tatranska Lomnica, High Tatras, June 2011

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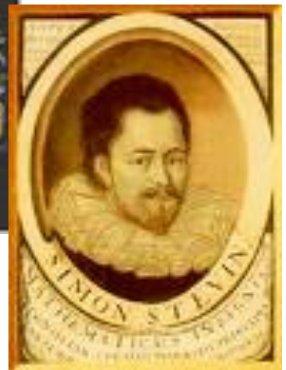
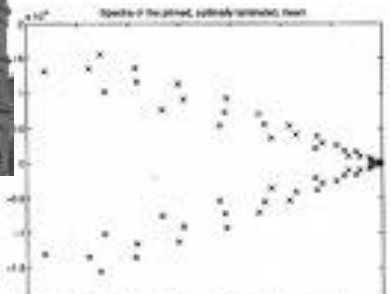
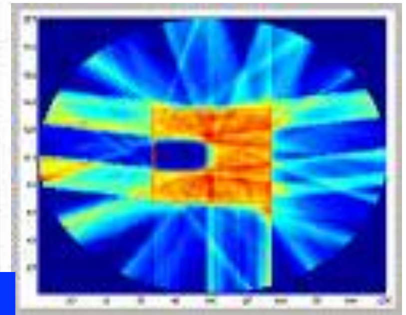
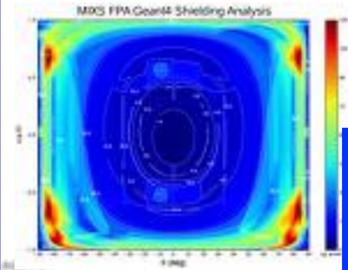
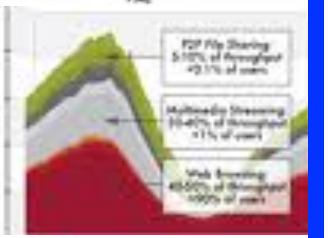


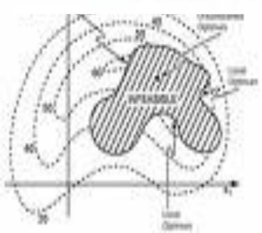
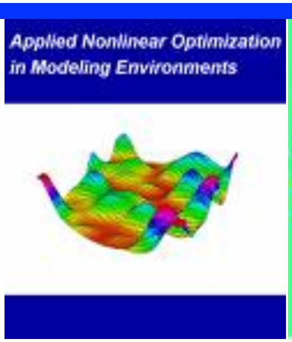





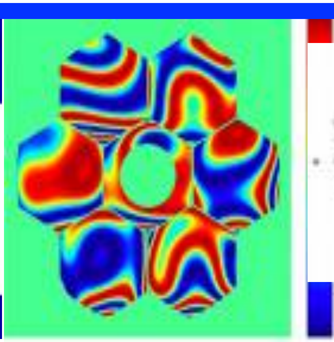
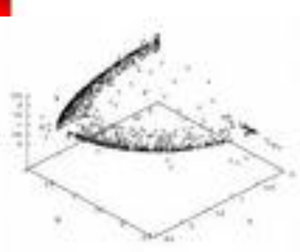
Optimization of process operation

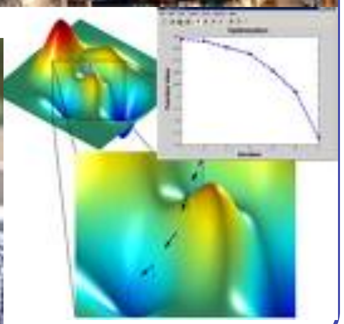
- Static optimization *u* — ***RTO***
  - dynamic processes at steady-state
  - run-to-run operation of batch processes

- Dynamic optimization *u(t)* — ***DRTO***
  - transient behavior of dynamic process





Outline

Context of uncertainty

- Plant-model mismatch
- Disturbances

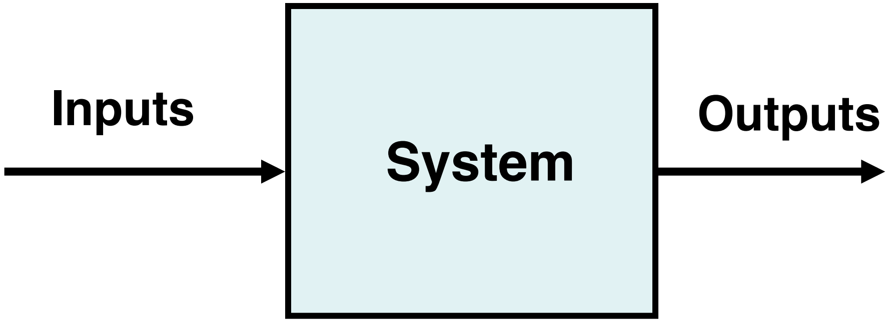
→ Use measurements for process improvement

Static real-time optimization

- *Adaptation of model parameters* – Repeated identification & optimization
- *Adaptation of optimization problem* – Modifier adaptation
- *Adaptation of inputs* – NCO tracking

Application examples

Control vs. Optimization

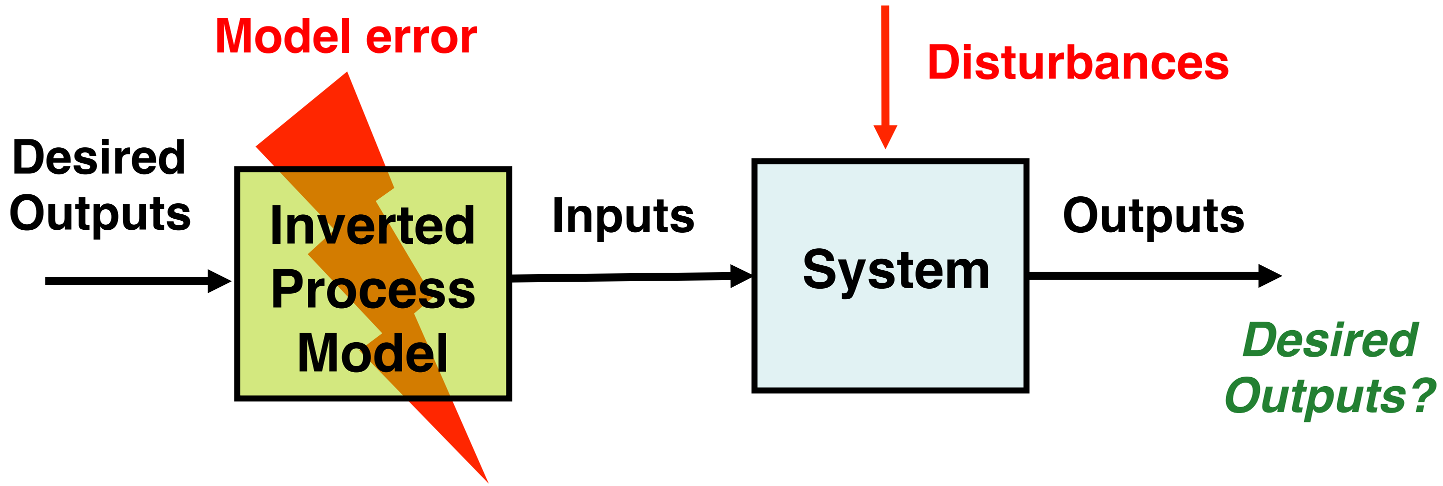


Control task:
What inputs should be applied to get the desired outputs ?

Optimization task:
What inputs should be applied to optimize the objective function ?

Control -- A Problem of Inversion

Inversion requires a process model (issue of causality)

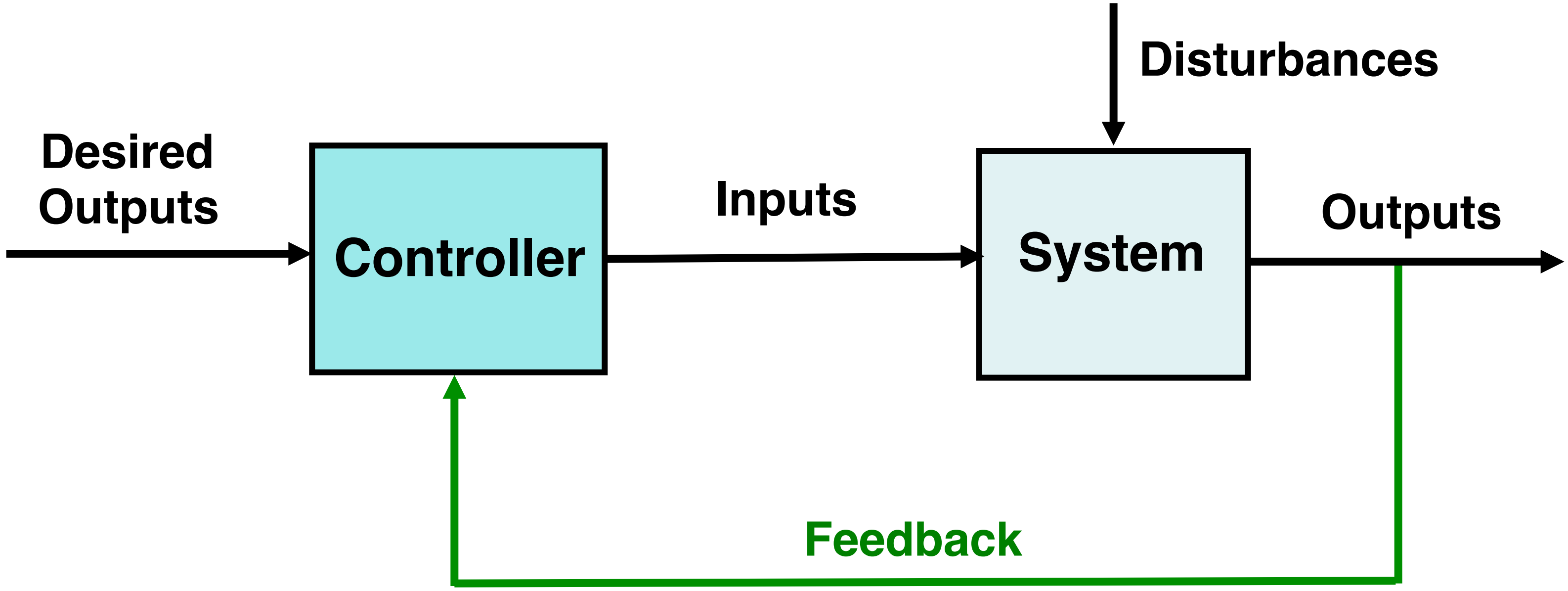


Approximate Inversion by Feedback

Use measurements to compensate uncertainty

Approximation of the inverse introduces robustness

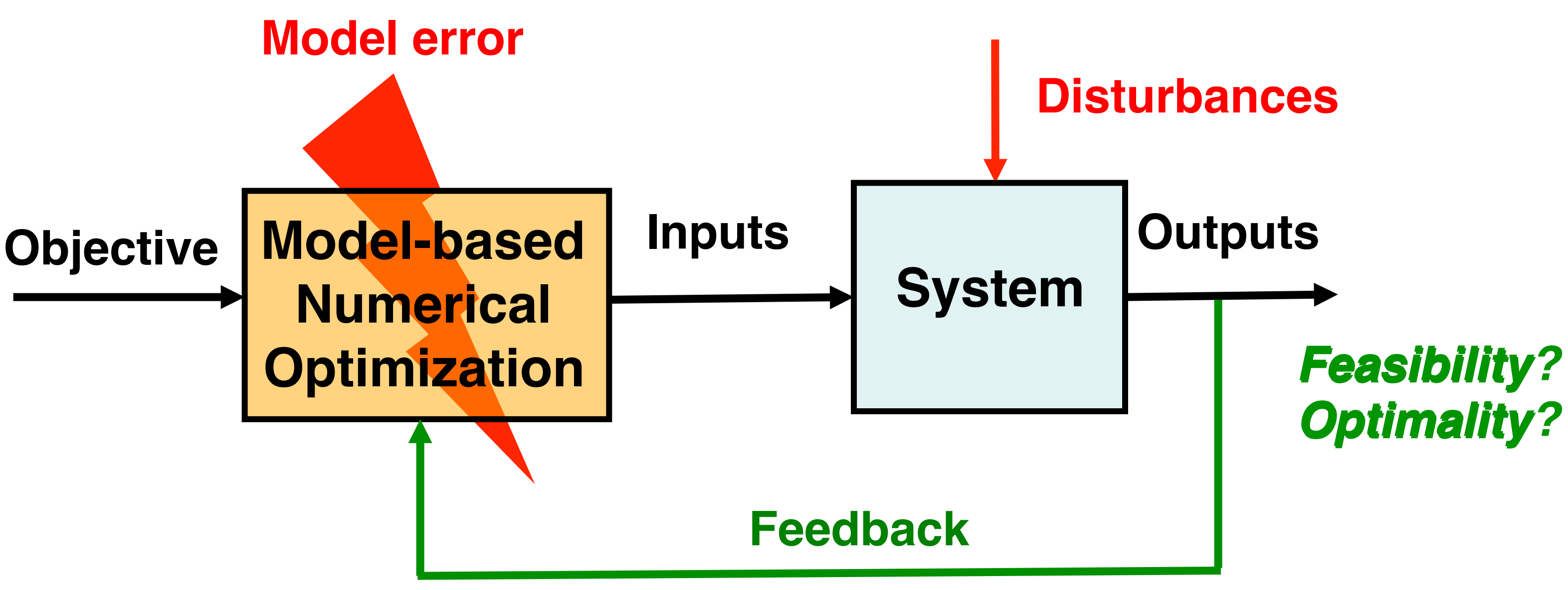
Controller ensures stability and tracking performance



Optimization

A Problem of "Best" Inversion

Numerical optimization using a process model



This talk: How to implement this feedback ?

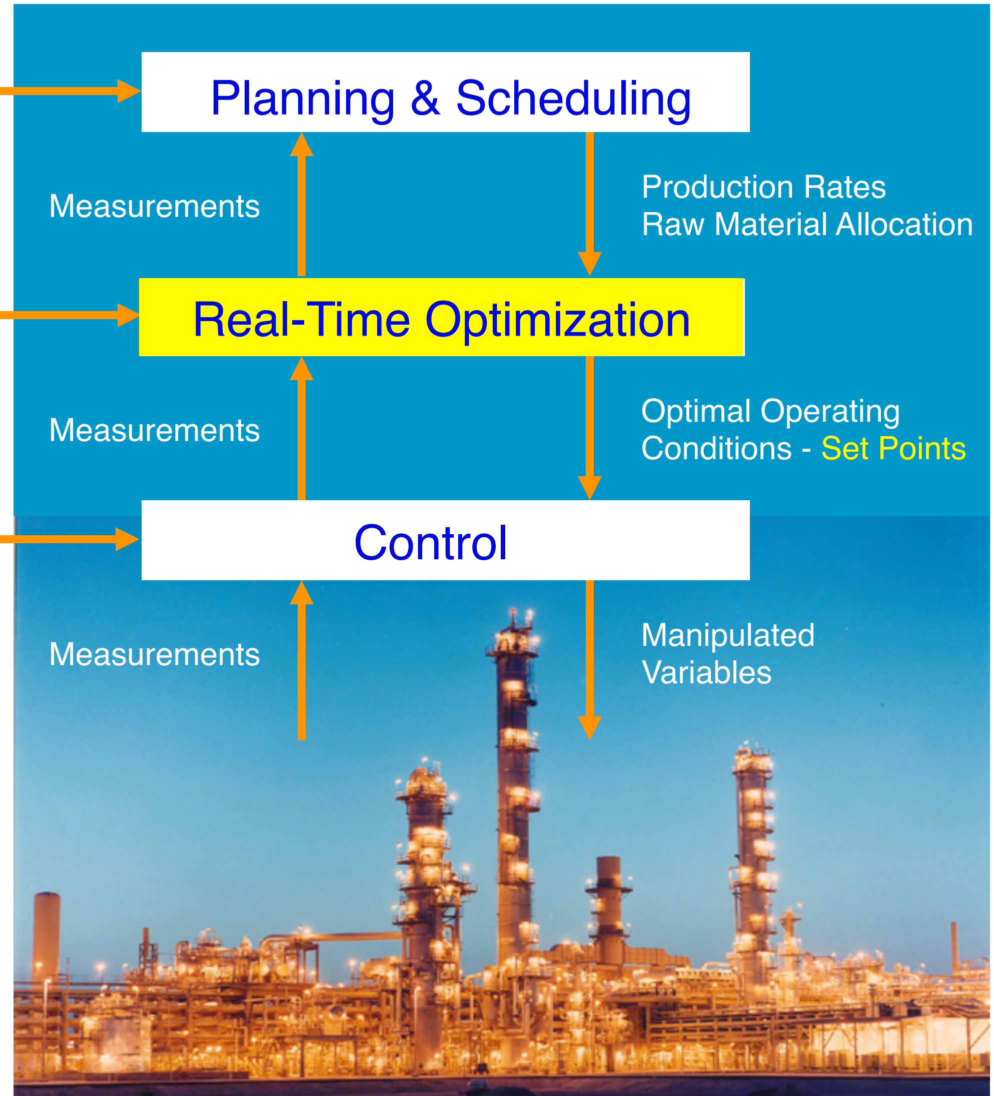
Real-Time Optimization of a Continuous Plant

	Disturbances
Long term week/month	Market Fluctuations, Demand, Price
Medium term day	Catalyst Decay, Changing Raw Material Quality
Short term second/minute	Fluctuations in Pressure, Flowrates, Compositions

Large-scale complex processes

Changing conditions
➔ Real-time adaptation

Decision Levels



Run-to-Run Optimization of a Batch Plant

$u(t)$ →  → $x_p(t_f)$

Batch plant with
finite terminal time

$$\min_{\mathbf{u}[0,t_f]} \quad \Phi := \phi\left(\mathbf{x}(t_f), \boldsymbol{\theta}\right)$$

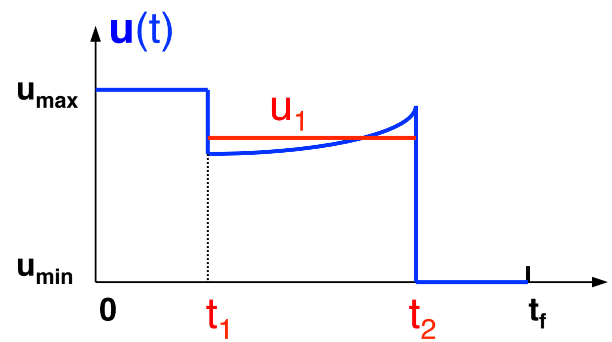
$$\text{s.t.} \quad \dot{\mathbf{x}} = \mathbf{F}(\mathbf{x}, \mathbf{u}, \boldsymbol{\theta}) \quad \mathbf{x}(0) = \mathbf{x}_0$$

$$\mathbf{S}(\mathbf{x}, \mathbf{u}, \boldsymbol{\theta}) \leq \mathbf{0}$$

$$\mathbf{T}\left(\mathbf{x}(t_f), \boldsymbol{\theta}\right) \leq \mathbf{0}$$

Input Parameterization

$$u[0, t_f] = U(\pi)$$



π →  → Φ_p, $\mathbf{G}_p$

Batch plant
viewed as a static map

$$\min_{\pi} \quad \Phi(\boldsymbol{\pi}, \boldsymbol{\theta})$$

$$\text{s.t.} \quad \mathbf{G}(\boldsymbol{\pi}, \boldsymbol{\theta}) \leq \mathbf{0}$$

NLP

Static RTO Problem

Minimize some steady-state performance (e.g. cost),
while satisfying a number of operating constraints (e.g. safety)

Plant

$$\min_{\mathbf{u}} \quad \Phi_p(\mathbf{u}) := \phi_p(\mathbf{u}, \mathbf{y}_p)$$

$$\text{s. t.} \quad \mathbf{G}_p(\mathbf{u}) := \mathbf{g}_p(\mathbf{u}, \mathbf{y}_p) \leq \mathbf{0}$$

Model-based Optimization

$$\mathbf{F}(\mathbf{u}, \mathbf{y}, \boldsymbol{\theta}) = \mathbf{0}$$

$$\min_{\mathbf{u}} \quad \Phi(\mathbf{u}) := \phi(\mathbf{u}, \mathbf{y})$$

$$\text{s. t.} \quad \mathbf{G}(\mathbf{u}) := \mathbf{g}(\mathbf{u}, \mathbf{y}) \leq \mathbf{0}$$

NLP

Inputs $\mathbf{u}$?

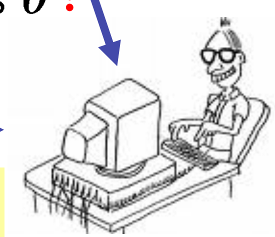
(set points)

Plant Outputs $\mathbf{y_p}$

Model Parameters $\boldsymbol{\theta}$?

Inputs $\mathbf{u}$?

(set points)



Predicted Outputs $\mathbf{y}$

RTO Scenarios

Optimization in the presence of Uncertainty

$$
\begin{aligned}
\mathbf{u}^* \in \arg\min_{\mathbf{u}} \quad & \phi(\mathbf{u},\mathbf{y}) \\
\text{s.t.} \quad & \mathbf{F}(\mathbf{u},\mathbf{y},\boldsymbol{\theta}) = \mathbf{0} \\
& \mathbf{g}(\mathbf{u},\mathbf{y}) \leq \mathbf{0}
\end{aligned}
$$

- input update: $\delta\mathbf{u}$
- parameter update: $\delta\boldsymbol{\theta}$
- constraint update: $\delta\mathbf{g}$

What are the best **handles** for correction?

No Measurement:
Robust Optimization

Measurements:
Adaptive Optimization

Adaptation of Model Parameters	Adaptation of KKT Modifiers	Adaptation of Inputs
- repeated identification and optimization	*- bias update*	*- tracking active constraints*
- two-step approach	*- constraint update*	*- NCO tracking*
	- gradient correction	*- extremum-seeking control*
	- ISOPE	*- self-optimizing control*

1. Adaptation of Model Parameters

Repeated Identification and Optimization

Parameter Estimation Problem

$$\theta_k^* \in \arg\min_{\theta} \quad J_k^{\text{id}}$$

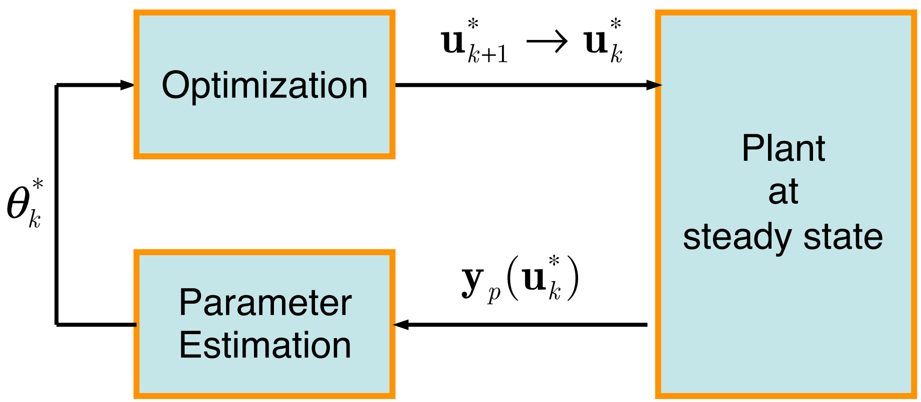
$$J_k^{\text{id}} = \left[\mathbf{y}_p(\mathbf{u}_k^*) - \mathbf{y}(\mathbf{u}_k^*, \theta)\right]^{\mathrm{T}} \mathrm{Q} \left[\mathbf{y}_p(\mathbf{u}_k^*) - \mathbf{y}(\mathbf{u}_k^*, \theta)\right]$$

Optimization Problem

$$\mathbf{u}_{k+1}^* \in \arg\min_{\mathbf{u}} \quad \phi\left(\mathbf{u}, \mathbf{y}(\mathbf{u}, \theta_k^*)\right)$$

$$\text{s.t.} \quad \mathbf{g}\left(\mathbf{u}, \mathbf{y}(\mathbf{u}, \theta_k^*)\right) \leq \mathbf{0}$$

$$\mathbf{u}^{\mathrm{L}} \leq \mathbf{u} \leq \mathbf{u}^{\mathrm{U}}$$

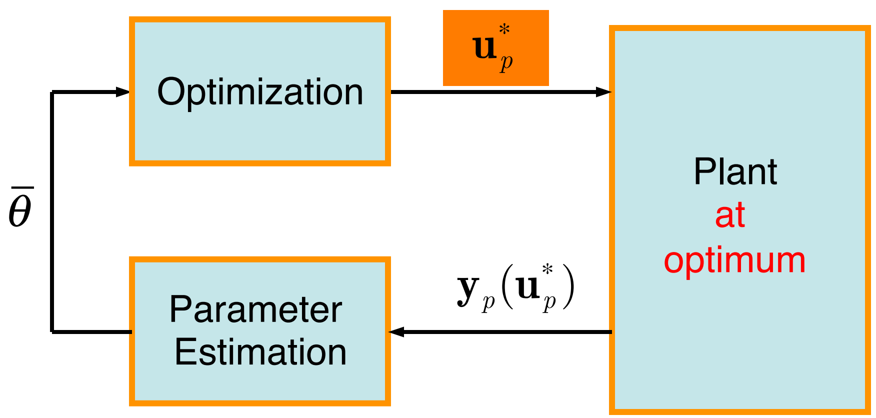


Current Industrial Practice
for tracking the changing optimum
in the presence of disturbances

T.E. Marlin, A.N. Hrymak. Real-Time Operations Optimization of Continuous Processes, *AIChE Symposium Series - CPC-V*, **93**, 156-164, 1997

Model Adequacy for Two-Step Approach

A process model is said to be adequate for use in an RTO scheme if it is capable of producing a fixed point for that RTO scheme at the plant optimum



$\bar{\theta}$ Converged value

Model-adequacy conditions

Par. Est. (SOSC):

$$\frac{\partial J^{\text{id}}}{\partial \theta}\left(\mathbf{y}_p(\mathbf{u}_p^*), \mathbf{y}(\mathbf{u}_p^*, \bar{\theta})\right) = \mathbf{0},$$

$$\frac{\partial^2 J^{\text{id}}}{\partial \theta^2}\left(\mathbf{y}_p(\mathbf{u}_p^*), \mathbf{y}(\mathbf{u}_p^*, \bar{\theta})\right) > 0,$$

Opt.:

$$G_i(\mathbf{u}_p^*, \bar{\theta}) = 0, \quad i \in A(\mathbf{u}_p^*)$$

$$G_i(\mathbf{u}_p^*, \bar{\theta}) < 0, \quad i \notin A(\mathbf{u}_p^*)$$

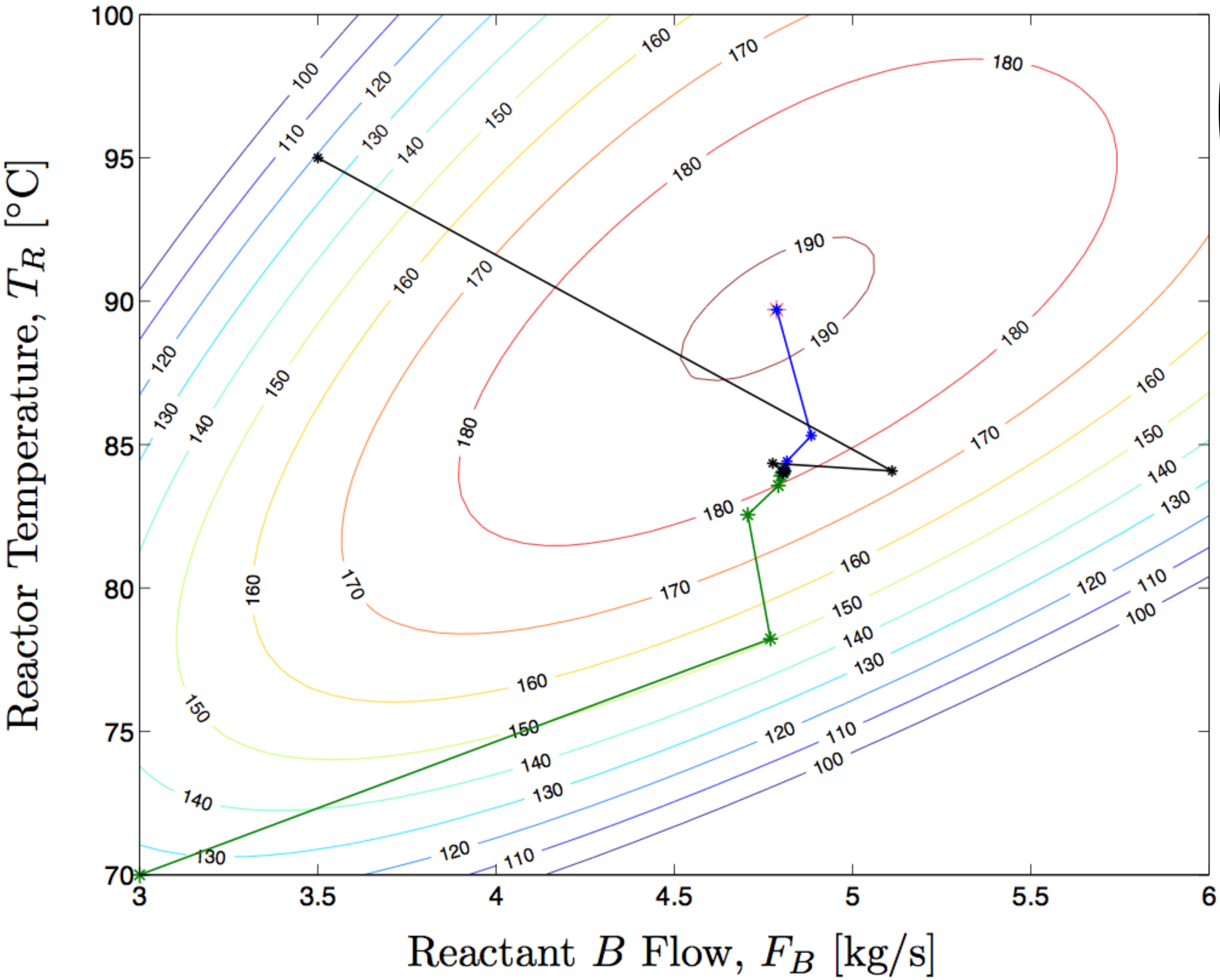
$$\nabla_r \Phi(\mathbf{u}_p^*, \bar{\theta}) = \mathbf{0},$$

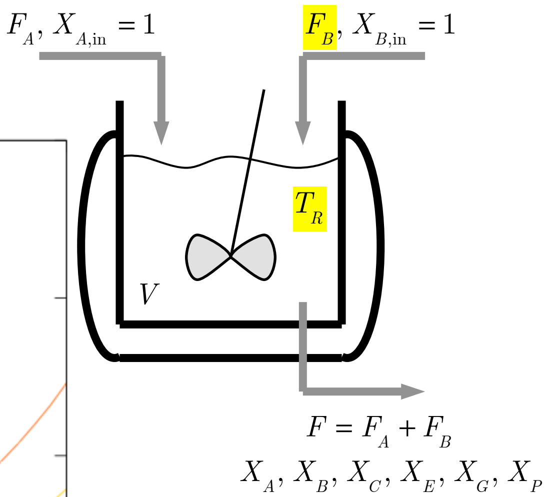
$$\nabla_r^2 \Phi(\mathbf{u}_p^*, \bar{\theta}) > 0$$

J.F. Forbes, T.E. Marlin. Design Cost: A Systematic Approach to Technology Selection for Model-Based Real-Time Optimization Systems. *Comp. Chem. Eng.*, **20**(6/7), 717-734, 1996

Example of Inadequate Model

Two-step approach





Williams-Otto Reactor

- 4^{th}-order model
- 2 inputs
- 2 adjustable par.

Does not convergence to plant optimum

2. Modification of Optimization Problem

Repeated Optimization using Nominal Model

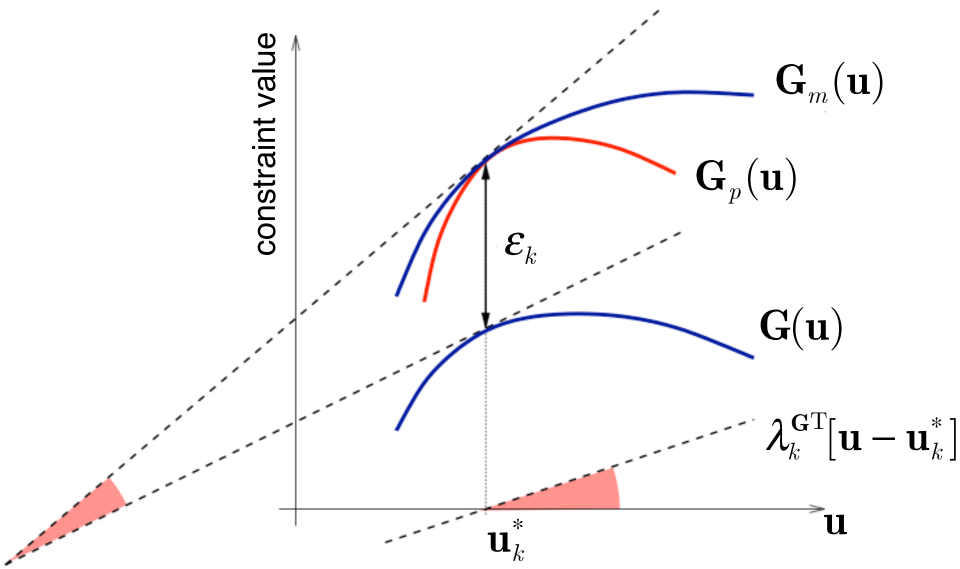
Modified Optimization Problem

$$\mathbf{u}_{k+1}^* \in \arg\min_{\mathbf{u}} \quad \Phi_m(\mathbf{u}) := \Phi(\mathbf{u}) + \lambda_k^{\Phi\mathrm{T}}[\mathbf{u} - \mathbf{u}_k^*]$$

$$\text{s.t.} \quad \mathbf{G}_m(\mathbf{u}) := \mathbf{G}(\mathbf{u}) + \varepsilon_k + \lambda_k^{\mathrm{GT}}[\mathbf{u} - \mathbf{u}_k^*] \le \mathbf{0}$$

$$\mathbf{u}^{\mathrm{L}} \le \mathbf{u} \le \mathbf{u}^{\mathrm{U}}$$

Affine corrections of cost and constraint functions



Force the modified problem to satisfy the optimality conditions of the **plant**

P.D. Roberts and T.W. Williams, On an Algorithm for Combined System Optimization and Parameter Estimation, *Automatica*, **17**(1), 199–209, 1981

2. Modification of Optimization Problem

Repeated Optimization using Nominal Model

Modified Optimization Problem

$$\mathbf{u}_{k+1}^* \in \arg\min_{\mathbf{u}} \quad \Phi_m(\mathbf{u}) := \Phi(\mathbf{u}) + \lambda_k^{\Phi\mathrm{T}}[\mathbf{u} - \mathbf{u}_k^*]$$

$$\text{s.t.} \quad \mathbf{G}_m(\mathbf{u}) := \mathbf{G}(\mathbf{u}) + \varepsilon_k + \lambda_k^{\mathbf{G}\mathrm{T}}[\mathbf{u} - \mathbf{u}_k^*] \leq \mathbf{0}$$

$$\mathbf{u}^{\mathrm{L}} \leq \mathbf{u} \leq \mathbf{u}^{\mathrm{U}}$$

- KKT Elements: $\mathcal{C}^{\mathrm{T}} = \left(G_1, \cdots, G_{n_g}, \frac{\partial G_1}{\partial \mathbf{u}}, \cdots, \frac{\partial G_{n_g}}{\partial \mathbf{u}}, \frac{\partial \Phi}{\partial \mathbf{u}} \right) \in \mathbb{R}^{n_K}$ $\quad n_K = n_g + n_u(n_g + 1)$
- KKT Modifiers: $\Lambda^{\mathrm{T}} = \left(\varepsilon_1, \cdots, \varepsilon_{n_g}, \lambda^{G_1 \mathrm{T}}, \cdots, \lambda^{G_{n_g} \mathrm{T}}, \lambda^{\Phi \mathrm{T}} \right) \in \mathbb{R}^{n_K}$

Modifier Update (without filter)

$$\Lambda_k = \mathrm{C}_p(\mathbf{u}_k^*) - \mathrm{C}(\mathbf{u}_k^*)$$

Requires evaluation of KKT elements of plant

Modifier Update (with filter)

$$\Lambda_k = (\mathbf{I} - \mathrm{K})\,\Lambda_{k-1} + \mathrm{K}\left[\mathrm{C}_p(\mathbf{u}_k^*) - \mathrm{C}(\mathbf{u}_k^*)\right]$$

W. Gao and S. Engell, Iterative Set-point Optimization of Batch Chromatography, *Comput. Chem. Eng.*, **29**, 1401–1409, 2005

A. Marchetti, B. Chachuat and D. Bonvin, Modifier-Adaptation Methodology for Real-Time Optimization, I&EC Research, **48**(13), 6022-6033 (2009)

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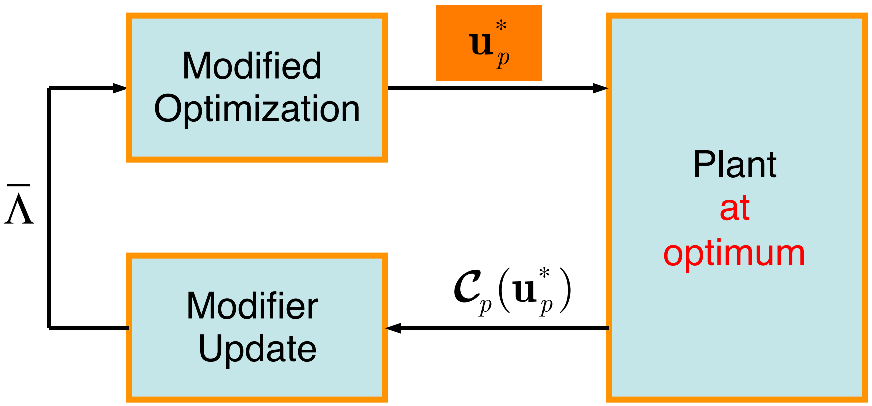

$\bar{\Lambda} = \mathcal{C}_p(\mathbf{u}_p^*) - \mathcal{C}(\mathbf{u}_p^*)$ Converged value

Model-adequacy condition

$$\frac{\partial J^{\rm id}}{\partial \theta}\Big(\mathbf{y}_p(\mathbf{u}_p^*), \mathbf{y}(\mathbf{u}_p^*)\Big) = \mathbf{0},$$

$$\frac{\partial^2 J^{\rm id}}{\partial \theta^2}\Big(\mathbf{y}_p(\mathbf{u}_p^*), \mathbf{y}(\mathbf{u}_p^*)\Big) > 0$$

$$G_i(\mathbf{u}_p^*) = 0, \quad i \in A(\mathbf{u}_p^*)$$

$$G_i(\mathbf{u}_p^*) < 0, \quad i \notin A(\mathbf{u}_p^*)$$

$$\nabla_r \Phi(\mathbf{u}_p^*) = \mathbf{0},$$

$$\nabla_r^2 \Phi(\mathbf{u}_p^*, \bar{\Lambda}) > 0$$

Example Revisited

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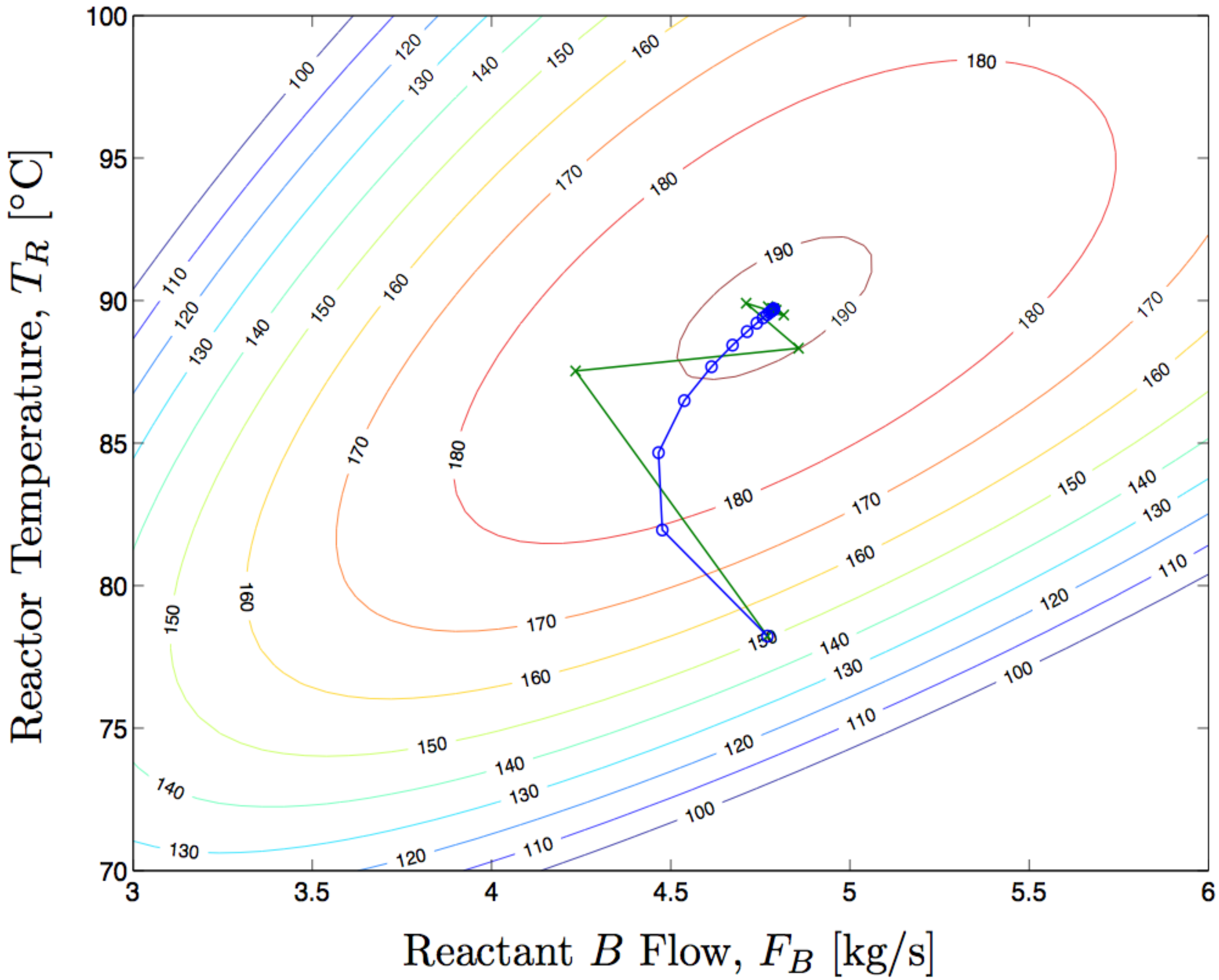
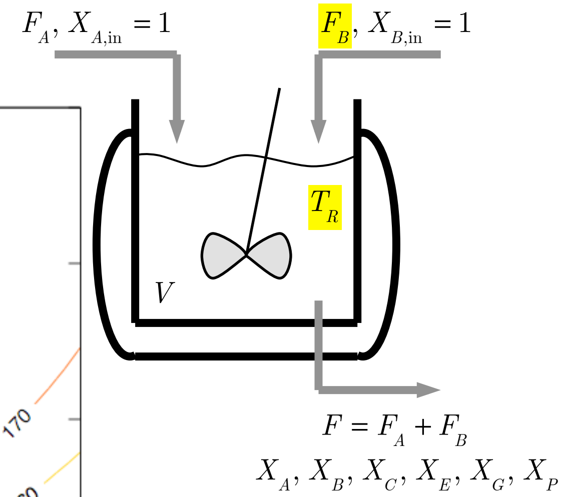
Modifier adaptation





Williams-Otto Reactor

- 4^{th}-order model
- 2 inputs
- 2 adjustable par.

Converges to plant optimum

Alejandro Marchetti, PhD thesis, EPFL, Modifier-Adaptation Methodology for Real-Time Optimization, 2009

3. Adaptation of Inputs NCO tracking

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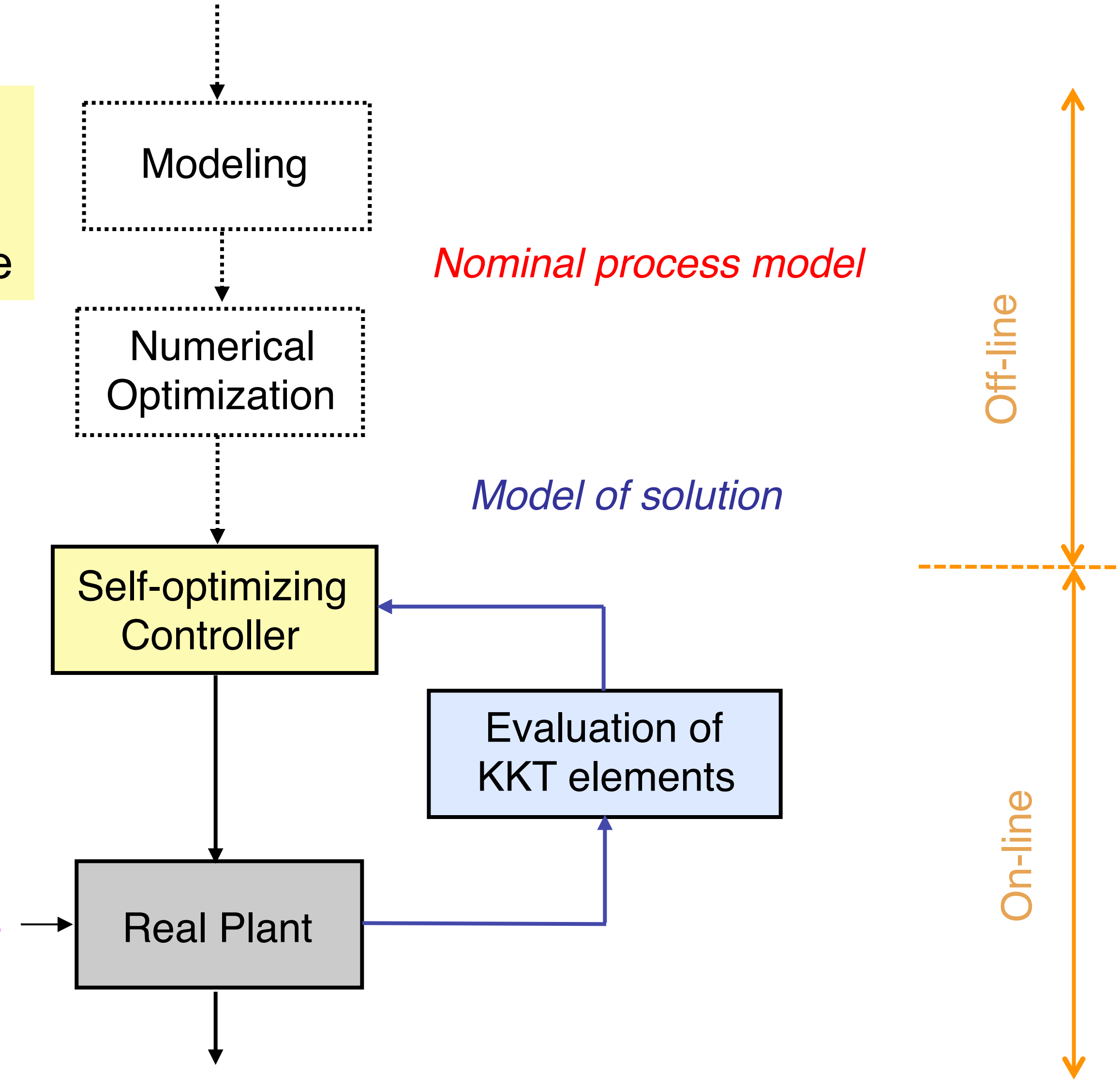
Self-optimizing control
→ no need to repeat
numerical optimization on-line

Active constraints
Reduced gradients



B. Srinivasan and D. Bonvin, Real-Time Optimization of Batch Processes by Tracking the Necessary Conditions of Optimality, *I&EC Research*, 46(2), 492-504, 2007

Outline

Context of uncertainty

→ Plant-model mismatch

→ Use of measurements for process improvement

Static real-time optimization (process at steady-state)

- *Adaptation of model parameters* – Repeated identification & optimization
- *Adaptation of optimization problem* – Modifier adaptation
- *Adaptation of inputs* – NCO tracking

Application examples

Comparison of 3 RTO Schemes

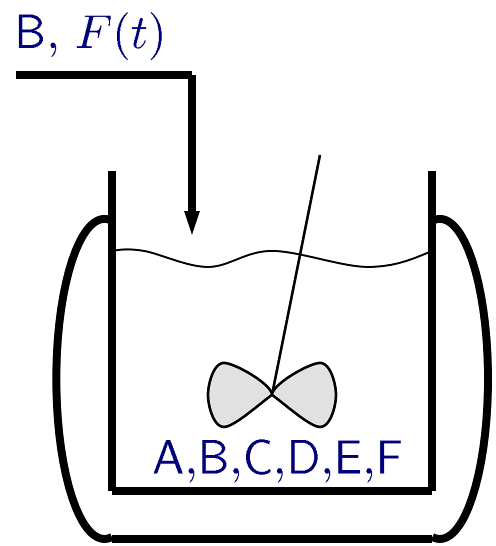
Run-to-Run Optimization of Semi-Batch Reactor

- **Industrial Reaction System** Lonza

$$\mathrm{A} + \mathrm{B} \xrightarrow{k_1} \mathrm{C}$$
$$2\mathrm{B} \xrightarrow{k_2} \mathrm{D}$$
$$\mathrm{B} \xrightarrow{k_3} \mathrm{E}$$
$$\mathrm{C} + \mathrm{B} \xrightarrow{k_4} \mathrm{F}$$

Simulated Reality

Model



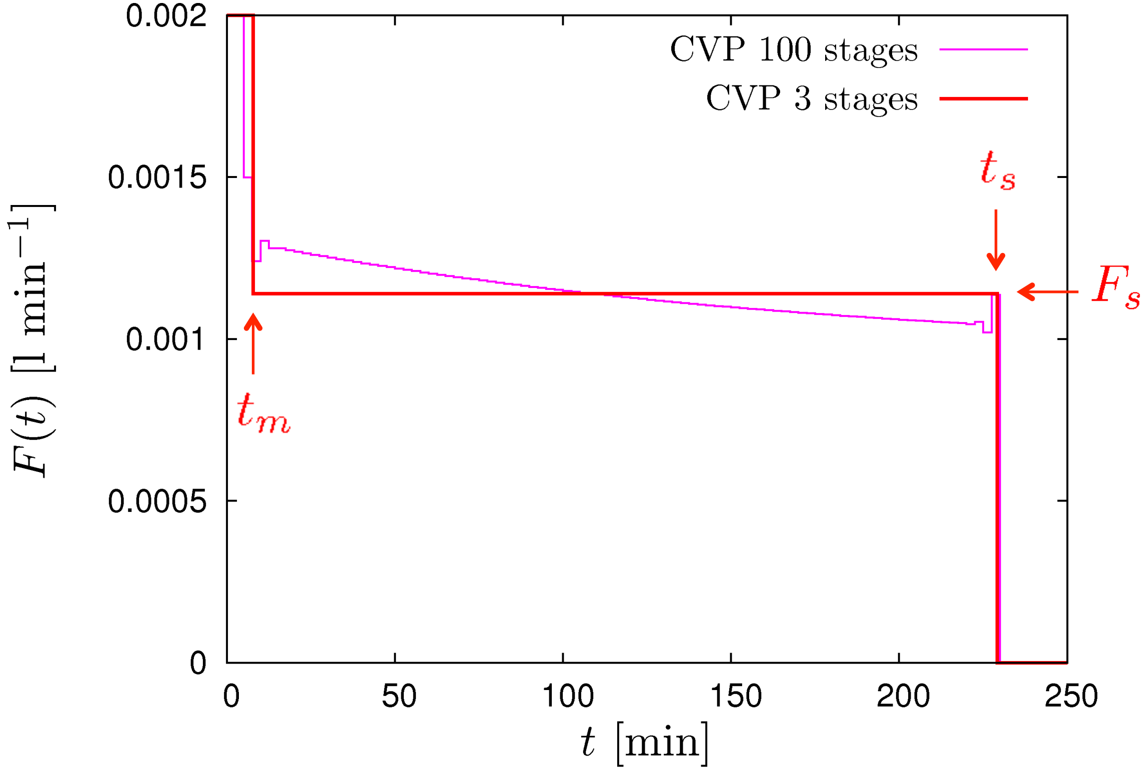
- Manipulated Variables: $F(t)$ (feed flow rate of B)
- Objective: Maximize $n_C(t_f)$ (production of C)
- Constraints:

Input bounds: $0 \leq F(t) \leq 0.002 \text{ l min}^{-1}$

Terminal constraints: $c_B(t_f) \leq 0.025 \text{ mol l}^{-1}$ (max. residual concentration)

$c_D(t_f) \leq 0.15 \text{ mol l}^{-1}$ (max. by-product concentration)

Nominal Input Trajectory



- **Optimal Solution**

  3 arcs, 2 active terminal constraints

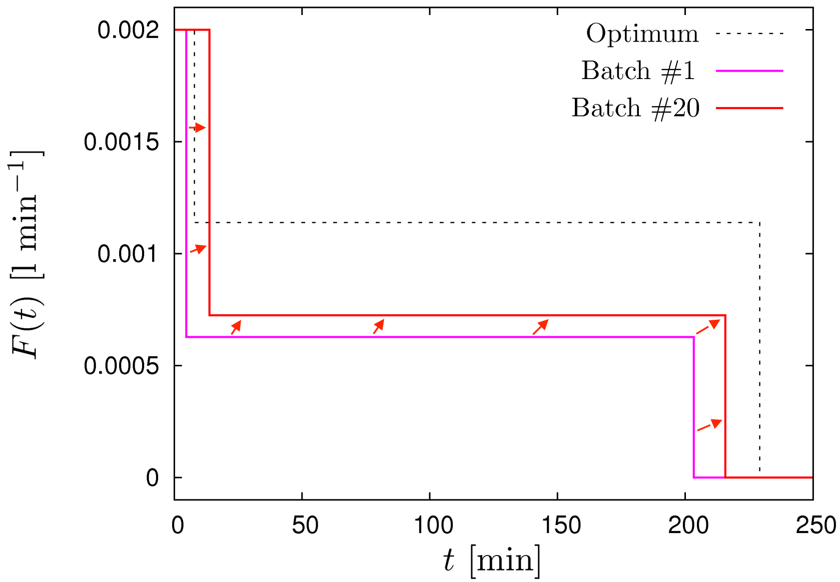
  $J^\star \approx 0.5081$ mol

- **Approximate Solution**

  Parameterization: $\mathbf{u} = (t_m, t_s, F_s)$

  $J^\star \approx 0.5079$ mol

Adaptation of Model Parameters k_1 and k_2



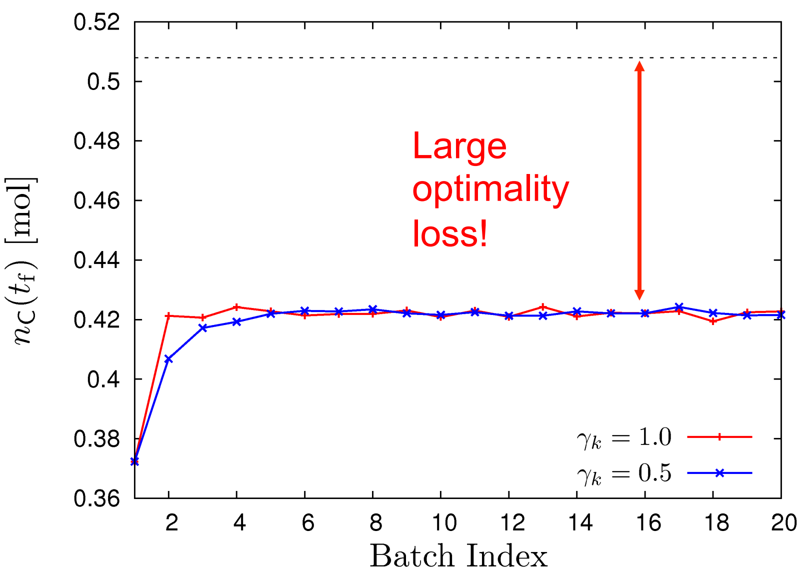
- Measurement Noise: $\sigma_y = 5\%$
  (10% constraint backoffs)

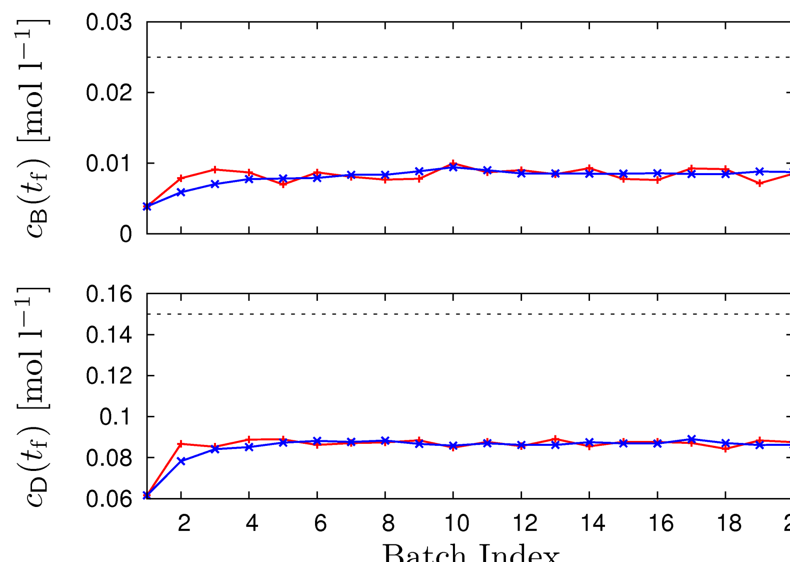
- Identification Objective:

$$J^{\text{id}} = \sum_{k=1}^{n^{\text{meas}}} \left[\frac{y - y^{\text{meas}}}{\bar{y}} \right]^2_{t=t_k}, \quad y = (c_{\mathsf{B}}, c_{\mathsf{C}}, c_{\mathsf{D}}), \quad n^{\text{meas}} = 6$$

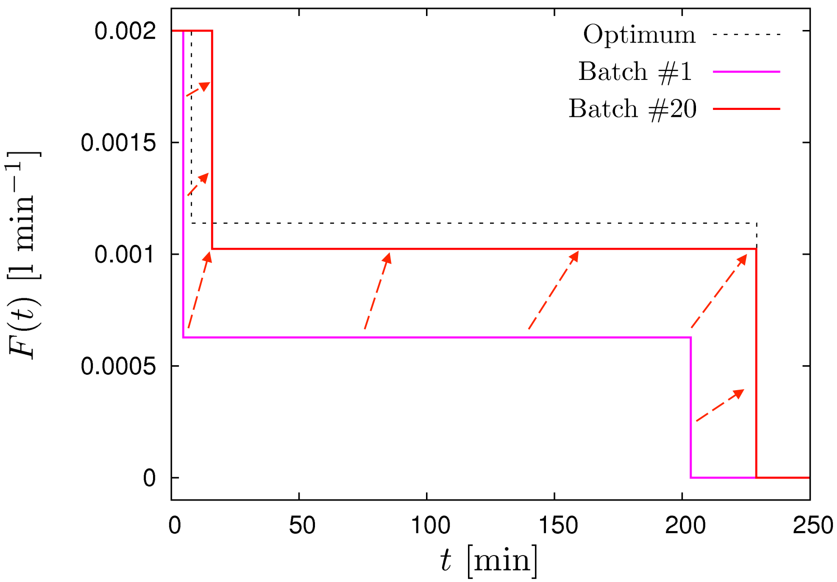
- Exponential Filter for k_1, k_2:

$$\begin{pmatrix} k_1^i \\ k_2^i \end{pmatrix} = (1 - \gamma_k) \begin{pmatrix} k_1^{i-1} \\ k_2^{i-1} \end{pmatrix} + \gamma_k \begin{pmatrix} k_1^\star \\ k_2^\star \end{pmatrix}$$



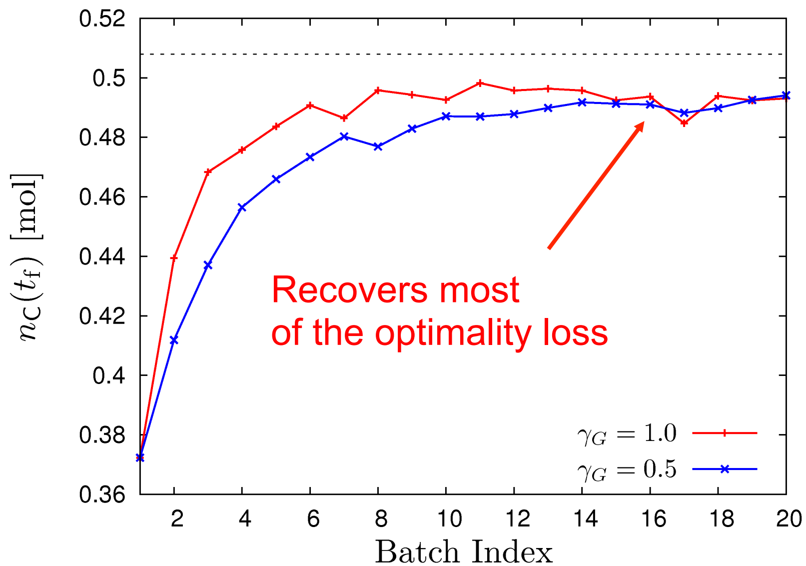


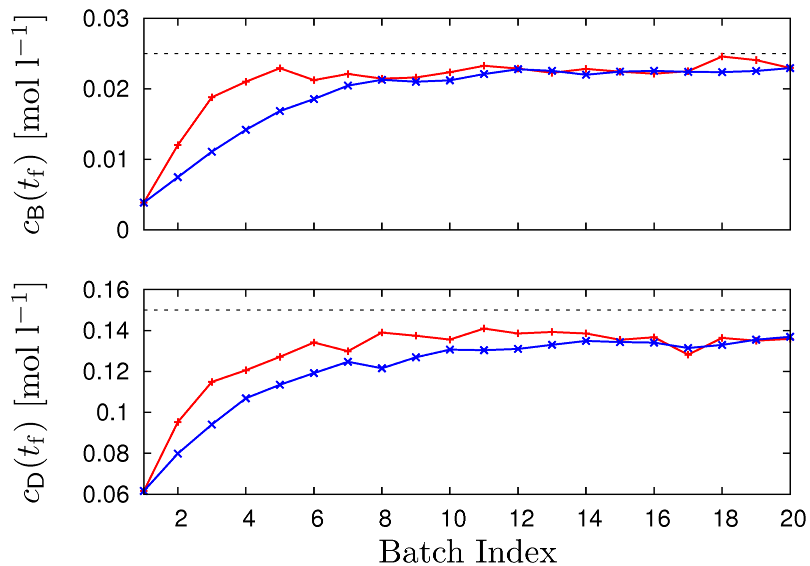
Adaptation of Modifiers ε_G



- Measurement Noise: $\sigma_y = 5\%$
  (10% constraint backoffs)
- No Gradient Correction
- Exponential Filter for Modifiers:

$$\begin{pmatrix} \varepsilon^i_{G,1} \\ \varepsilon^i_{G,2} \end{pmatrix} = (1-\gamma_G) \begin{pmatrix} \varepsilon^{i-1}_{G,1} \\ \varepsilon^{i-1}_{G,2} \end{pmatrix} + \gamma_G \begin{pmatrix} c^{\text{meas}}_{\text{B}}(t_{\text{f}}) - c_{\text{B}}(t_{\text{f}}) \\ c^{\text{meas}}_{\text{D}}(t_{\text{f}}) - c_{\text{D}}(t_{\text{f}}) \end{pmatrix}_{\boldsymbol{\pi}=\boldsymbol{\pi}^{i-1}}$$





Adaptation of Input Parameters t_s and F_s

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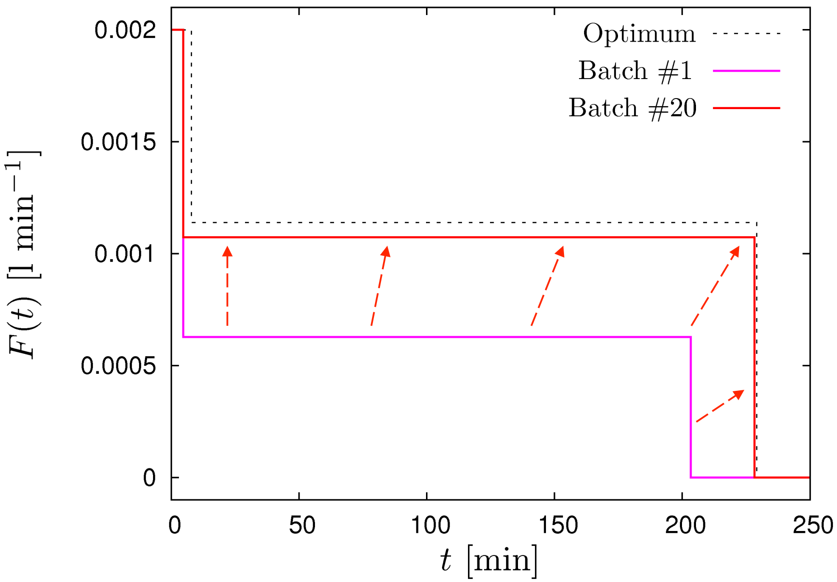
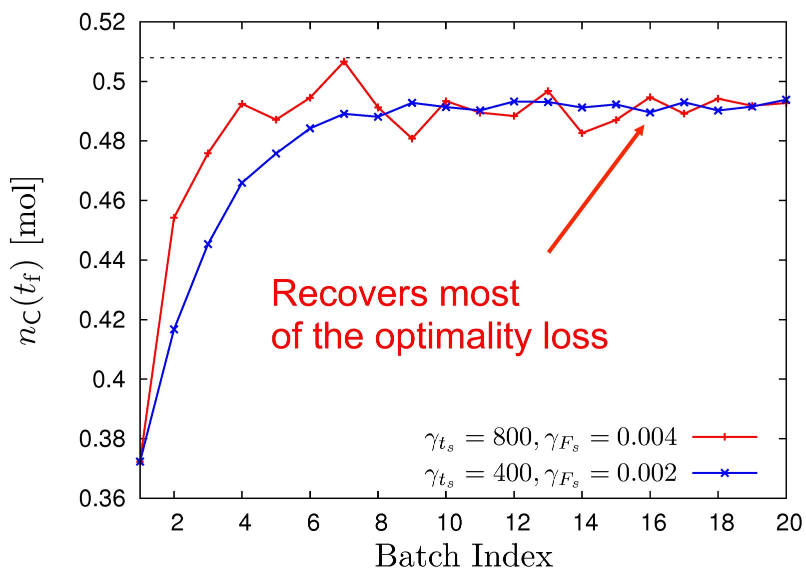
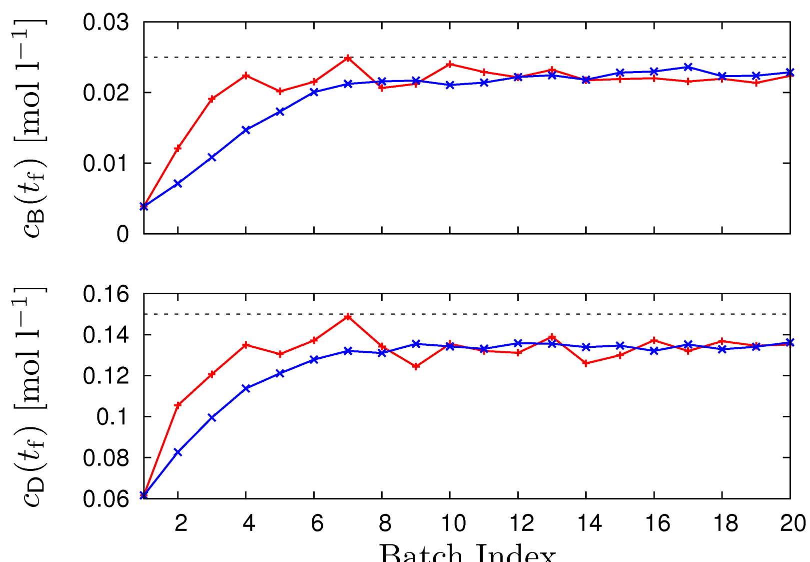


- Measurement Noise: $\sigma_y = 5\%$
  (10% constraint back-offs)
- No Gradient Correction
- Controller Design:

$$t_m = 4.71 \text{ min (fixed)}$$

$$\begin{pmatrix} t_s^k \\ F_s^k \end{pmatrix} = \begin{pmatrix} t_s^{k-1} \\ F_s^{k-1} \end{pmatrix} + \begin{pmatrix} \gamma_{t_s} & \\ & \gamma_{F_s} \end{pmatrix} \begin{pmatrix} c_B^{meas}(t_f) - 0.025 \\ c_D^{meas}(t_f) - 0.15 \end{pmatrix}_{\pi = \pi^{k-1}}$$





Industrial Application of NCO Tracking

Emulsion Copolymerization Process

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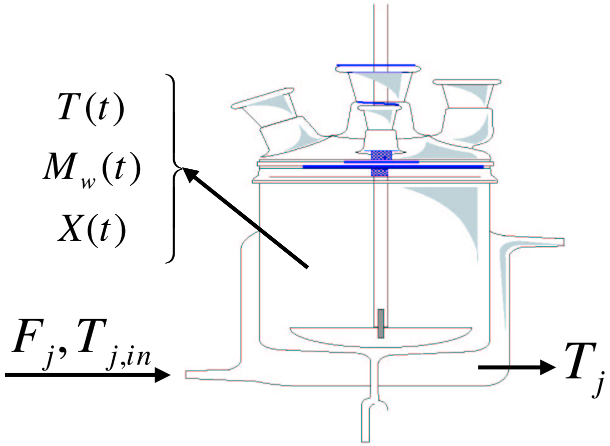
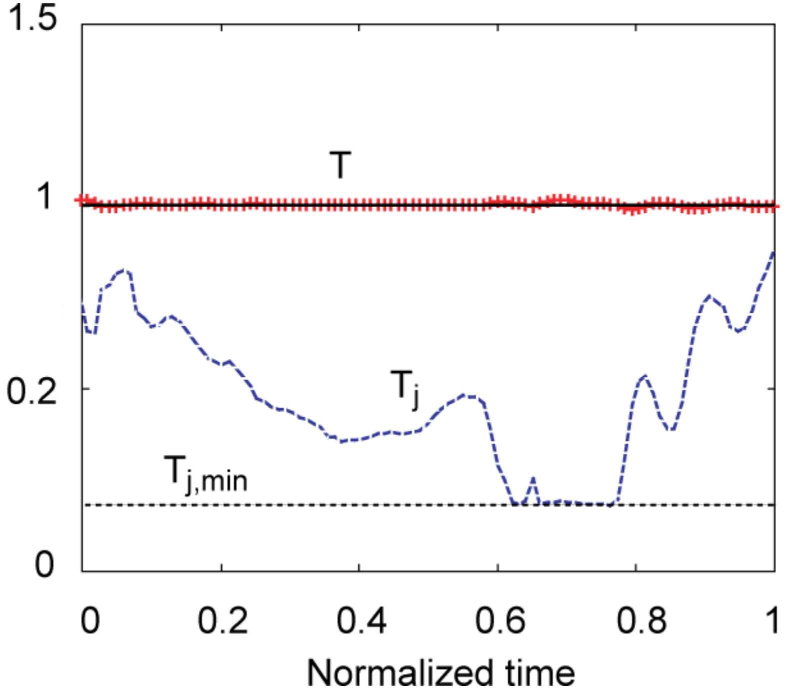
- Industrial features
  - 1-ton reactor, risk of runaway
  - Initiator efficiency can vary considerably
  - Several recipes
    - *different initial conditions*
    - *different initiator feeding policies*
    - *use of chain transfer agent*

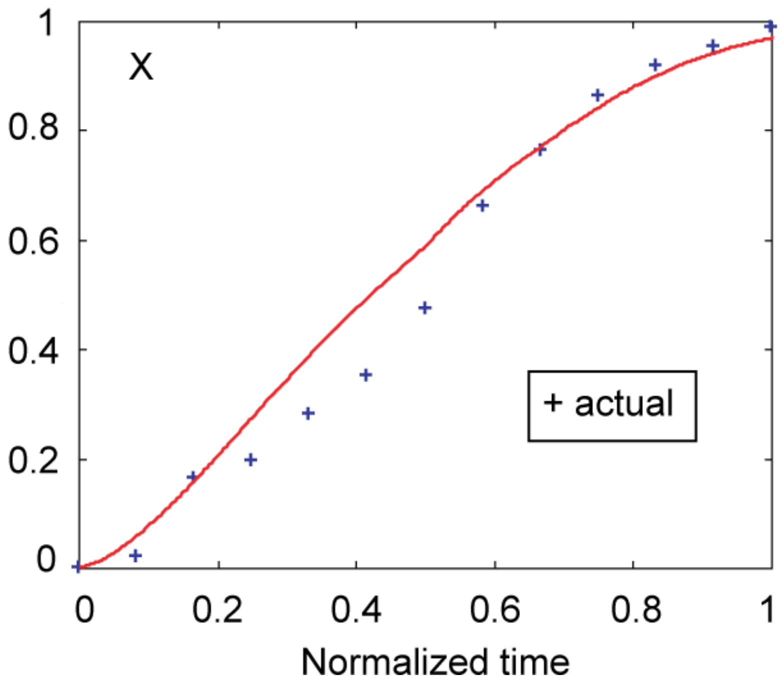


- Modeling difficulties
- Uncertainty

- Objective: Minimize batch time by adjusting the reactor temperature
  - Temperature and heat removal constraints
  - Quality constraints at final time

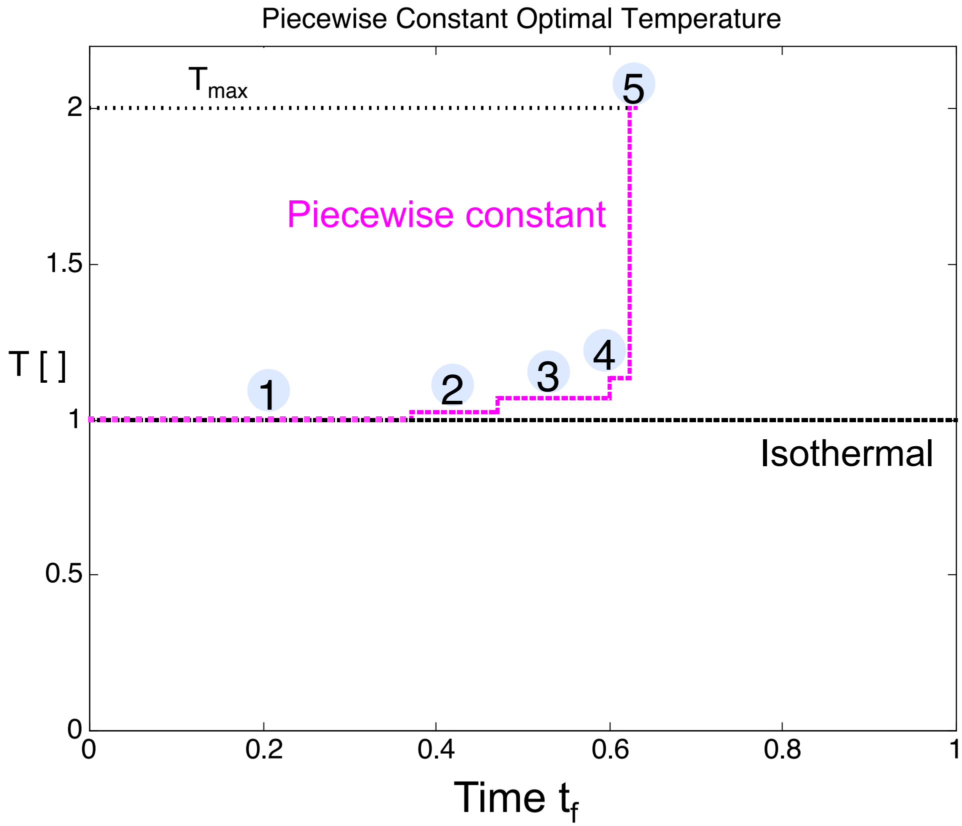
Industrial Practice





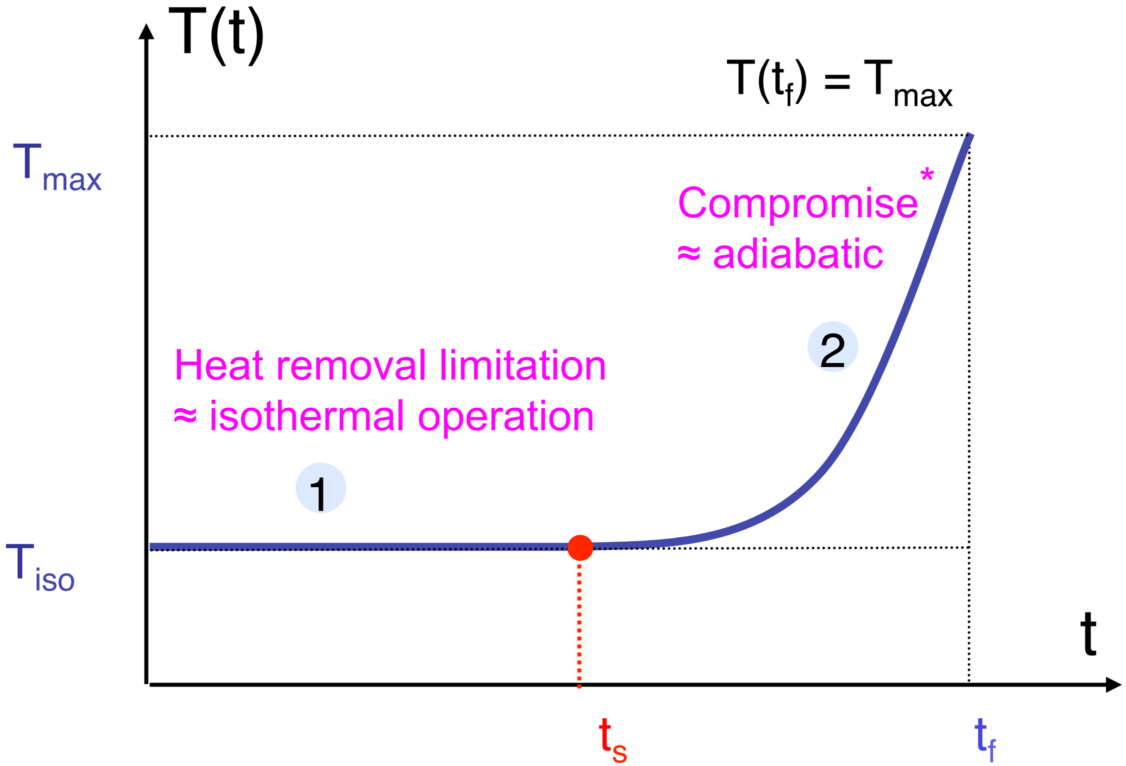
Optimal Temperature Profile

Numerical Solution using a Tendency Model



- Current practice: isothermal
- Numerical optimization
  - ✓ Piecewise-constant input
  - ✓ 5 decision variables (T_2-T_5, t_f)
  - ✓ Fixed relative switching times
- Active constraints
  - ✓ Interval 1: heat removal
  - ✓ Interval 5: T_{max}

Model of the Solution -- Semi-adiabatic Profile



*Compromise between conversion and quality

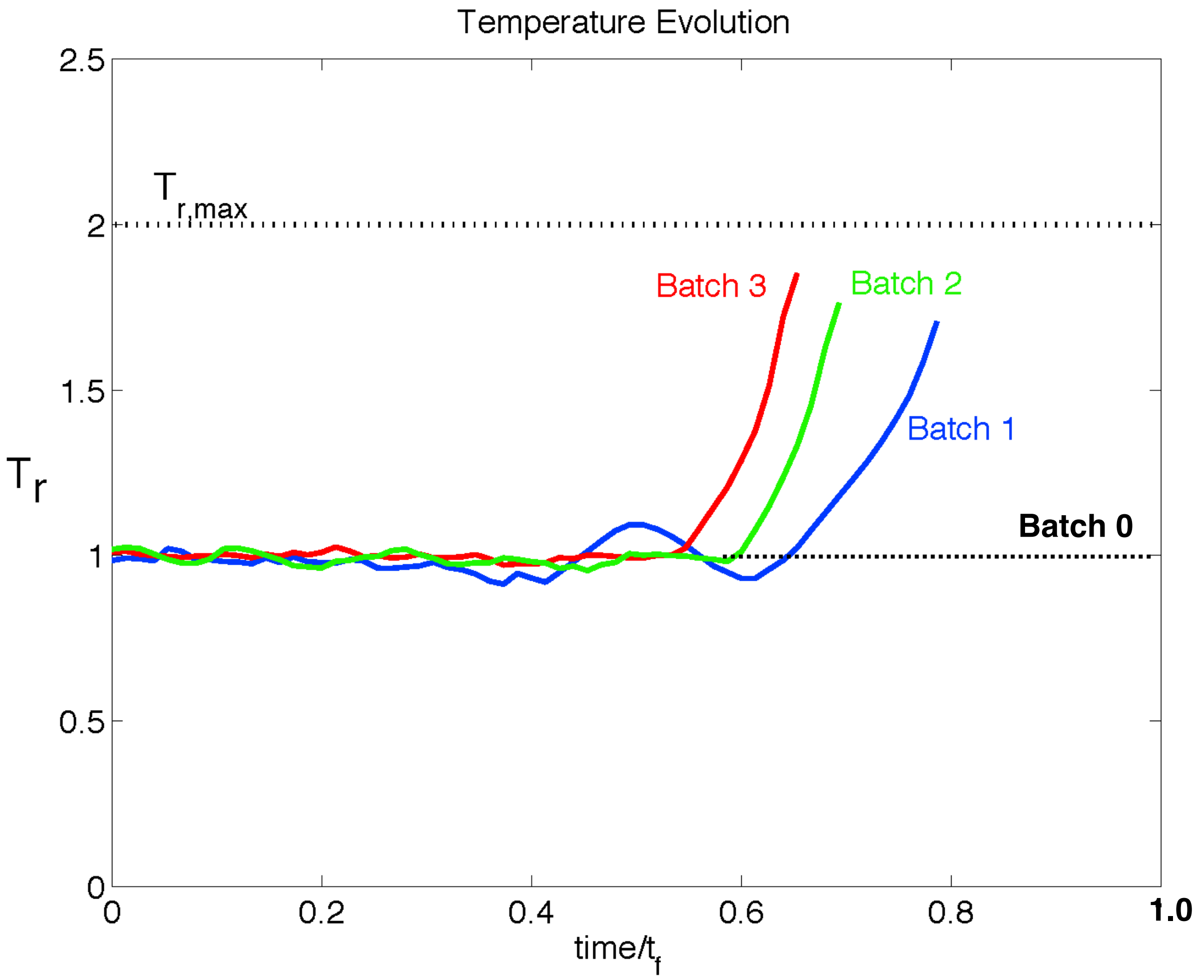
t_s enforces $T(t_f) = T_{max}$

Solution model → Fixed part -- structure

Solution model → Free part -- t_s

run-to-run adjustment of t_s

Industrial Results (1-ton reactor)



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Final time

- Isothermal: 1.00
- Batch 1: 0.78
- Batch 2: 0.72
- Batch 3: 0.65

Francois *et al.*, Run-to-run Adaptation of a Semi-adiabatic Policy for the Optimization of an Industrial Batch Polymerization Process, *I&EC Research*, **43**(23), 7238-7242, 2004

Conclusions

- Use measurements for process improvement
  - What is the best handle for correction?

- Repeated estimation and optimization can suffer from model-adequacy problem

- Practical observations
  - Complexity depends on the number of inputs (not system order)
  - Solution is often determined by the constraints of the problem

    → easy tracking