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Institute of Information Engineering, Automation, and Mathematics

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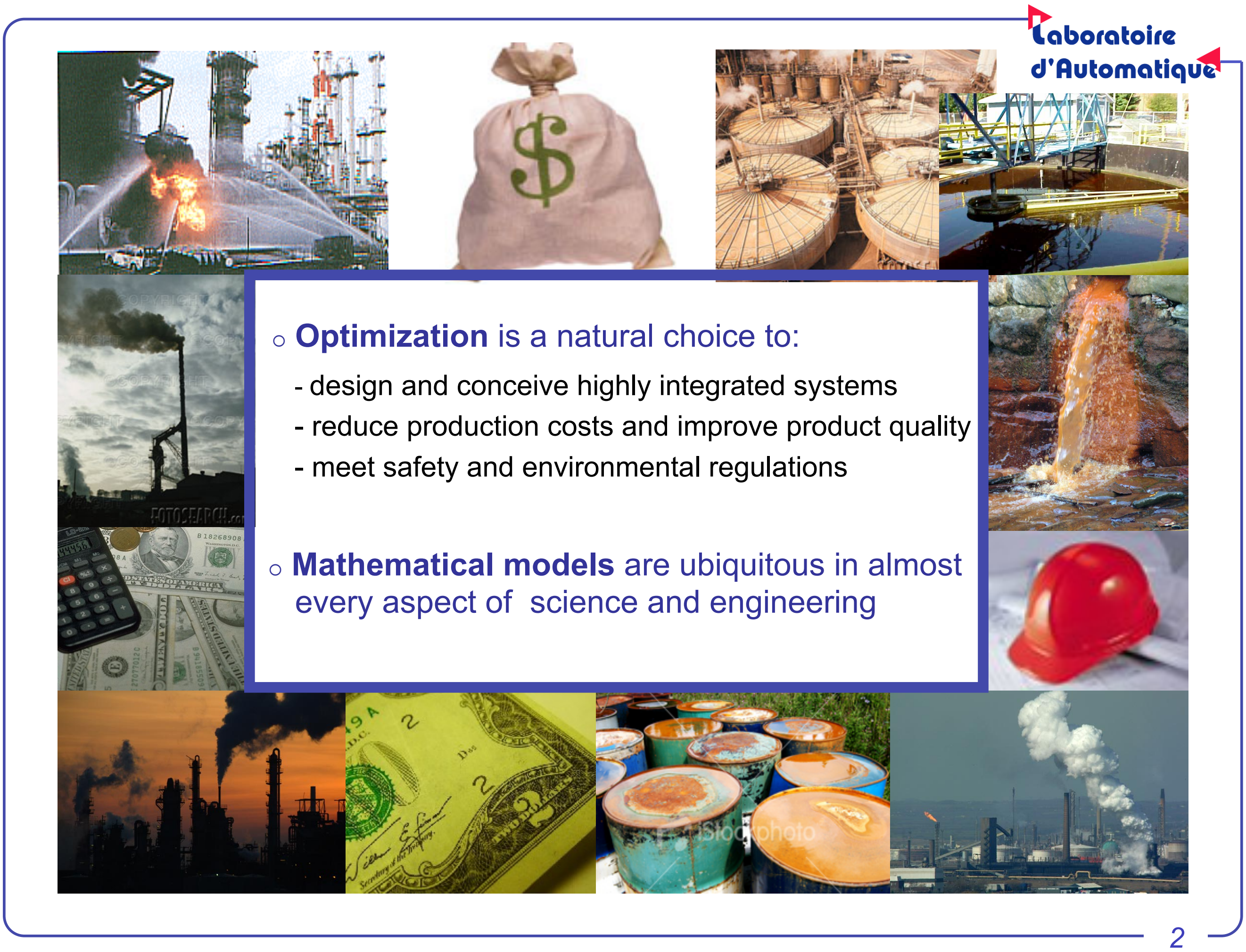
Full paper online: http://www.kirp.chtf.stuba.sk/pc11/data/abstracts/103.html

Real-Time Optimization in the Presence of Uncertainty

Dominique Bonvin
Laboratoire d'Automatique
EPFL, Lausanne

Process Control'11
Tatranska Lomnica, High Tatras, June 2011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d'Automatique
○ Optimization is a natural choice to:
- design and conceive highly integrated systems
- reduce production costs and improve product quality
- meet safety and environmental regulations
○ Mathematical models are ubiquitous in almost every aspect of science and engineering
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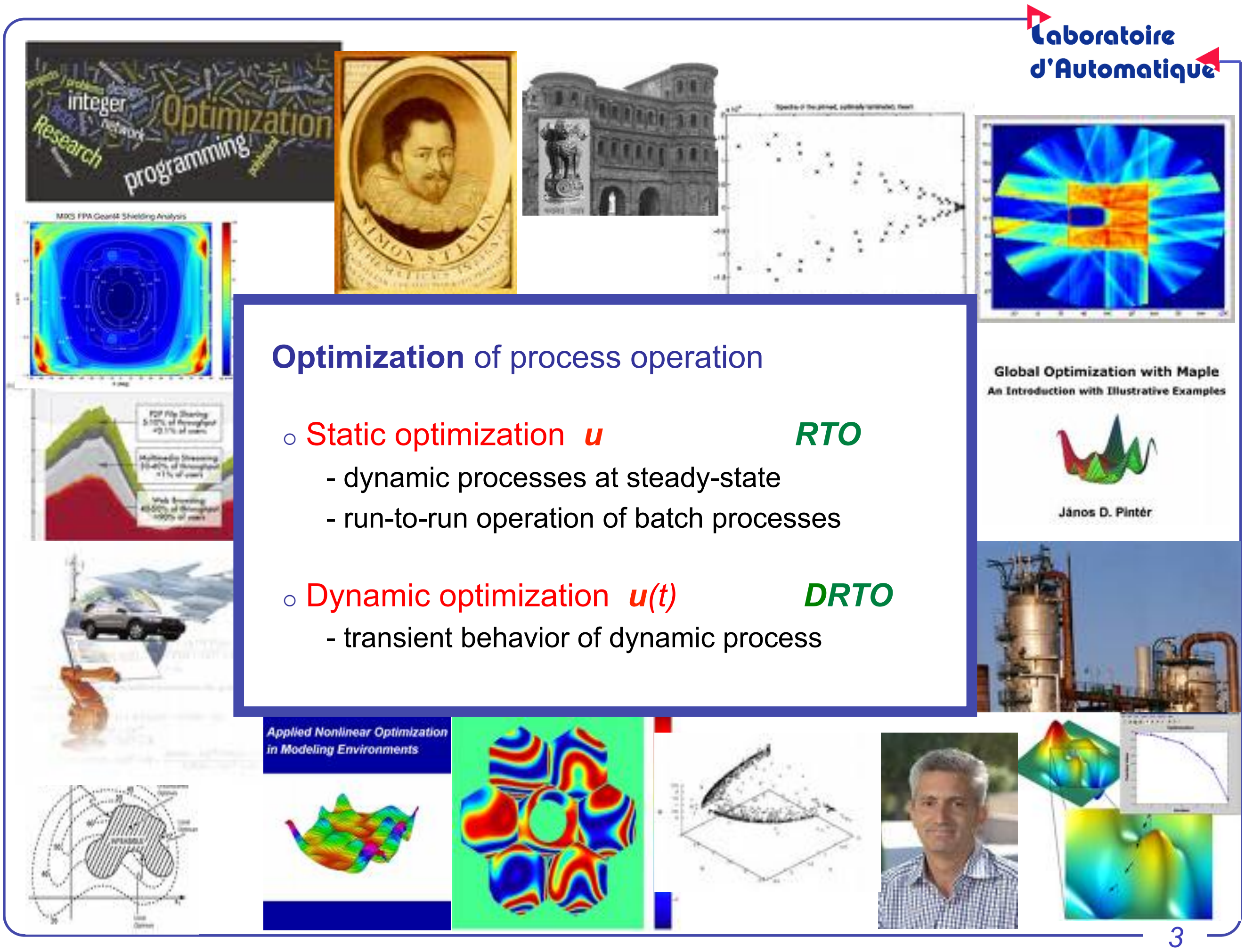
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integer
Optimization
Research
programming
Optimization of process operation
○ Static optimization u RTO
- dynamic processes at steady-state
- run-to-run operation of batch processes
○ Dynamic optimization u(t) DRTO
- transient behavior of dynamic process
Global Optimization with Maple
An Introduction with Illustrative Examples
János D. Pintér
Applied Nonlinear Optimization
in Modeling Environments
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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

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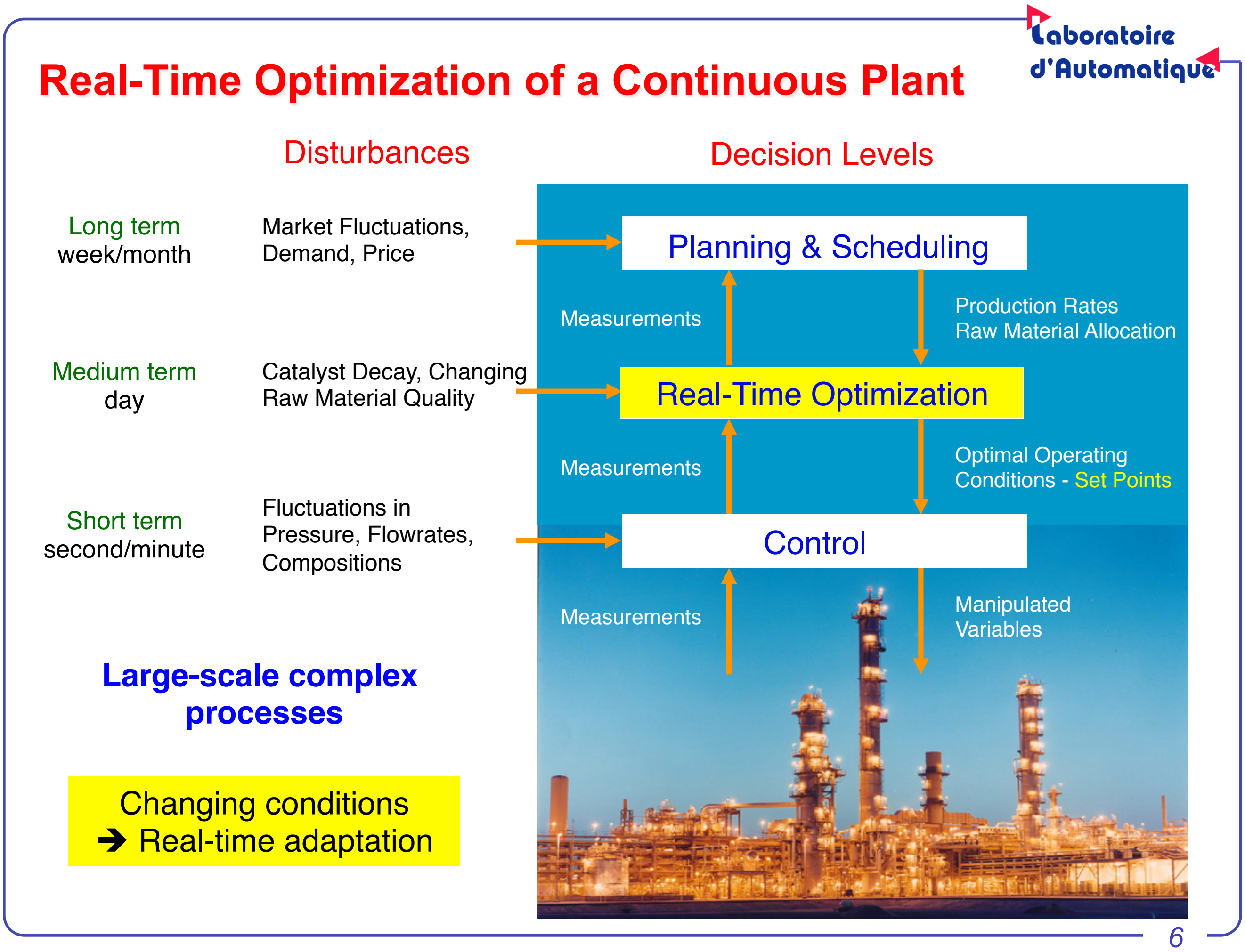
A Large Continuous Plant

5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Real-Time Optimization of a Continuous Plant
Disturbances
Decision Levels
Long term
week/month
Market Fluctuations,
Demand, Price
Planning & Scheduling
Measurements
Production Rates
Raw Material Allocation
Medium term
day
Catalyst Decay, Changing
Raw Material Quality
Real-Time Optimization
Measurements
Optimal Operating
Conditions - Set Points
Short term
second/minute
Fluctuations in
Pressure, Flowrates,
Compositions
Control
Measurements
Manipulated
Variables
Large-scale complex
processes
Changing conditions
➔ Real-time adaptation
6

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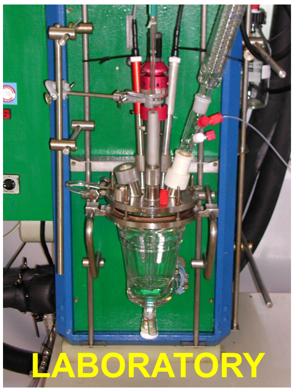
A Discontinous Plant

RECIPE → BATCH PLANT → PRODUCTS



Scale-up

Differences in Equipment and Scale

- mass- and heat-transfer characteristics
- surface-to-volume ratios
- operational constraints

Production Constraints

- meet product specifications
- meet safety and environmental constraints
- adhere to equipment constraints

Different conditions ➔ Run-to-run adaptation

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Run-to-Run Optimization of a Batch Plant

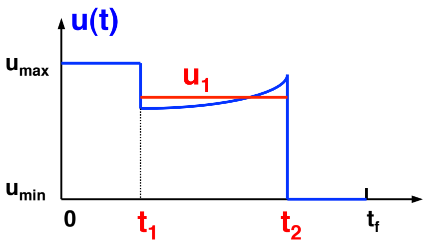
$u(t)$ →  → $x_p(t_f)$

Batch plant with finite terminal time

$$\min_{\mathbf{u}[0,t_f]} \quad \Phi := \phi\big(\mathbf{x}(t_f), \boldsymbol{\theta}\big)$$
$$\text{s.t.} \quad \dot{\mathbf{x}} = \mathbf{F}(\mathbf{x}, \mathbf{u}, \boldsymbol{\theta}) \quad \mathbf{x}(0) = \mathbf{x}_0$$
$$\mathbf{S}(\mathbf{x}, \mathbf{u}, \boldsymbol{\theta}) \le \mathbf{0}$$
$$\mathbf{T}\big(\mathbf{x}(t_f), \boldsymbol{\theta}\big) \le \mathbf{0}$$

Input Parameterization

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



π →  → Φ_p, $\mathbf{G}_p$

Batch plant viewed as a static map

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

NLP

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Static RTO Problem

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

Plant

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

Model-based Optimization

$$\mathbf{F}(\mathbf{u}, \mathbf{y}, \boldsymbol{\theta}) = \mathbf{0}$$
$$\min_{\mathbf{u}} \quad \Phi(\mathbf{u}) := \phi(\mathbf{u}, \mathbf{y})$$
$$\text{s.t.} \quad \mathbf{G}(\mathbf{u}) := \mathbf{g}(\mathbf{u}, \mathbf{y}) \le \mathbf{0}$$

NLP

Inputs $\mathbf{u}$?

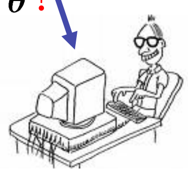
(set points)

Plant Outputs $\mathbf{y}_\mathbf{p}$

Model Parameters $\boldsymbol{\theta}$?

Inputs $\mathbf{u}$?

(set points)



Predicted Outputs $\mathbf{y}$

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RTO Scenarios

Optimization in the presence of Uncertainty

No Measurement: Robust Optimization

Measurements: Adaptive Optimization

input update: $\delta\mathbf{u}$

parameter update: $\delta\boldsymbol{\theta}$

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

constraint update: $\delta\mathbf{g}$

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

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

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1. Adaptation of Model Parameters

Repeated Identification and Optimization

Parameter Estimation Problem

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

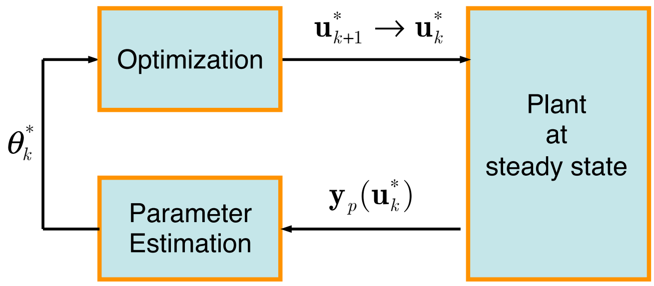
$$J_k^{\mathrm{id}} = \left[\mathbf{y}_p(\mathbf{u}_k^*) - \mathbf{y}(\mathbf{u}_k^*, \theta)\right]^{\mathrm{T}} \mathrm{Q} \left[\mathbf{y}_p(\mathbf{u}_k^*) - \mathbf{y}(\mathbf{u}_k^*, \theta)\right]$$

Optimization Problem

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

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

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



Current Industrial Practice
for tracking the changing optimum in
the presence of plant-model mismatch

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

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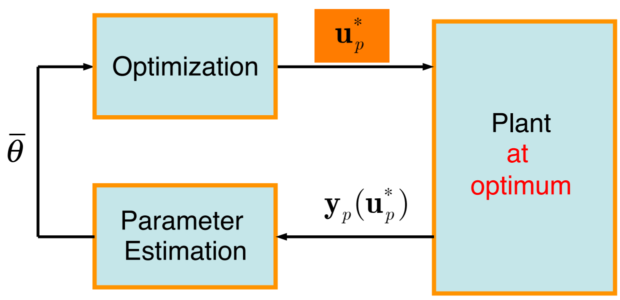
Model Adequacy for Two-Step Approach

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

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

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

SOSC

Par. Est.

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

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

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

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

Opt.

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

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Example of Inadequate Model

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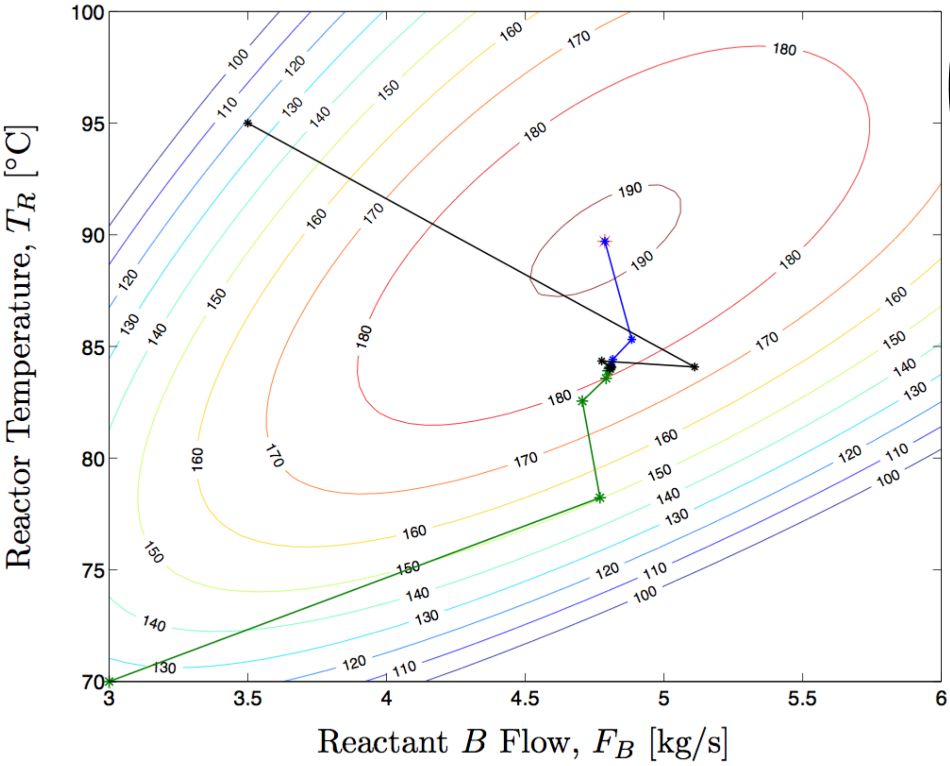
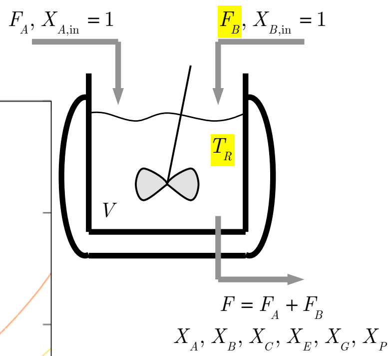
Two-step approach





Williams-Otto Reactor

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

Does not convergence to plant optimum

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2. Modification of Optimization Problem

Repeated Optimization using Nominal Model

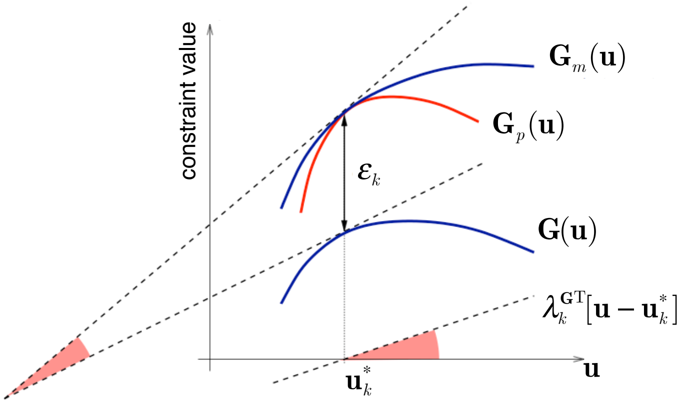
Modified Optimization Problem

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

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

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

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

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2. Modification of Optimization Problem

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Repeated Optimization using Nominal Model

Modified Optimization Problem

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

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

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

- KKT Elements: $$\mathcal{C}^{\mathrm{T}} = \left(G_1, \cdots, G_{n_g}, \frac{\partial G_1}{\partial \mathbf{u}}, \cdots, \frac{\partial G_{n_g}}{\partial \mathbf{u}}, \frac{\partial \Phi}{\partial \mathbf{u}} \right) \in \mathbb{R}^{n_K} \qquad n_K = n_g + n_u(n_g + 1)$$
- 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 for 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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Model Adequacy for Modifier Approach

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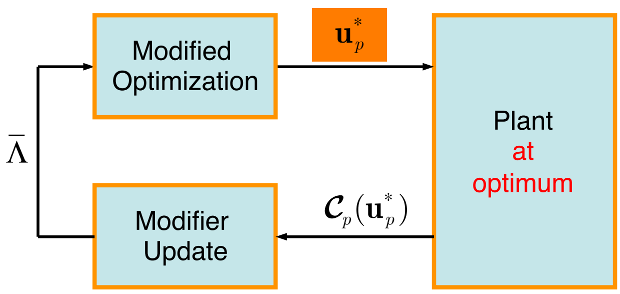
A process model is said to be adequate for use in an RTO scheme if it is capable of producing a fixed point for that RTO scheme at the plant optimum



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

Model-adequacy condition

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

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

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

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

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

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

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Example Revisited

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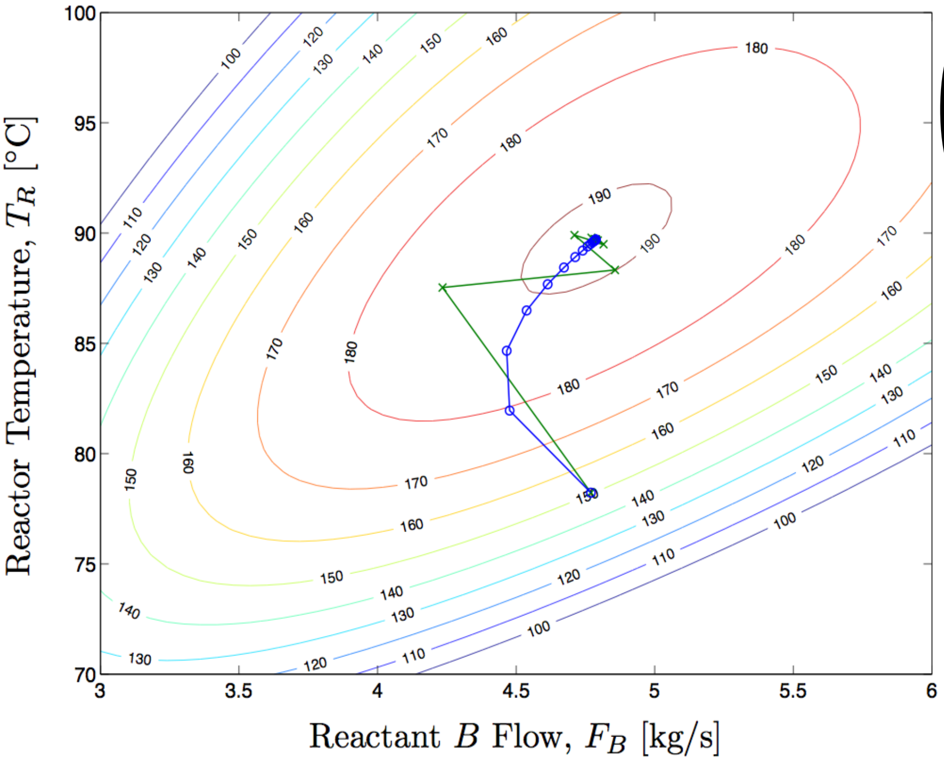
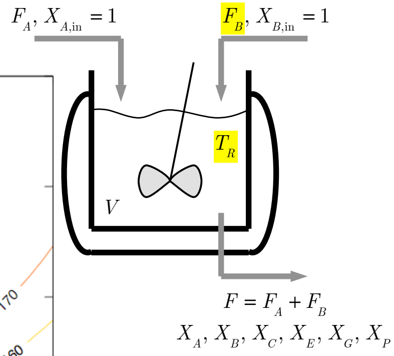
Modifier adaptation





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

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3. Adaptation of Inputs — NCO tracking

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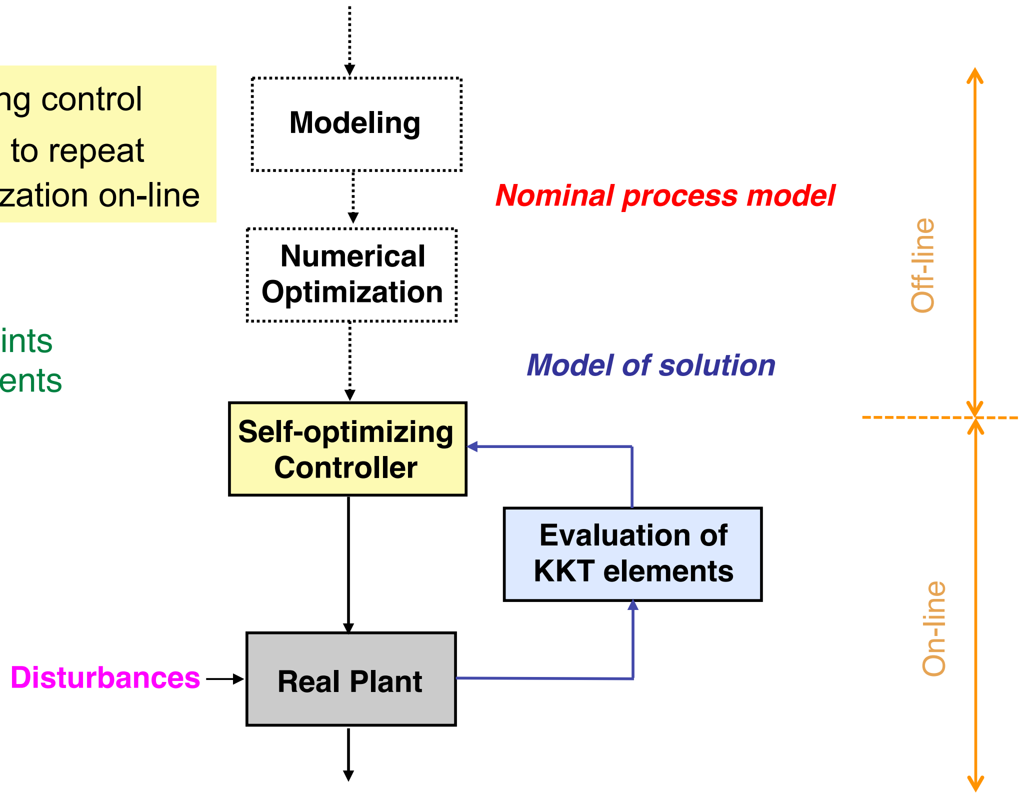
Self-optimizing control
→ no need to repeat
numerical optimization on-line

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

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Comparison of RTO Schemes

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	Model parameter adaptation	Modifier adaptation	Input adaptation (NCO tracking)
Adjustable parameters	$\boldsymbol{\theta}$	$\boldsymbol{\Lambda}$	$\mathbf{u}$
Measurements	$\mathbf{y}_p$	$\mathbf{C}_p$	$\mathbf{C}_p$
Number of parameters	n_θ	$n_g + n_u(n_g + 1)$	n_u
Number of measurements	n_y	$n_g + n_u(n_g + 1)$	$n_g + n_u(n_g + 1)$
On-line tasks	Optimization (2x)	Estimation of KKT Optimization	Estimation of KKT
Feasibility	✘ Constraints predicted by model	✔ Constraints measured	✔ OK if active set known
Optimality	✘ Gradients predicted by model	✔ Gradients measured	✔ Gradients measured
Strengths	Intuitive	One-to-one correspondence Constraint adaptation	No optimization on-line Constraint tracking
Weaknesses	Model adequacy	Experimental gradients	Knowledge of active set Experimental gradients Controller tuning

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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

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Comparison of 3 RTO Schemes

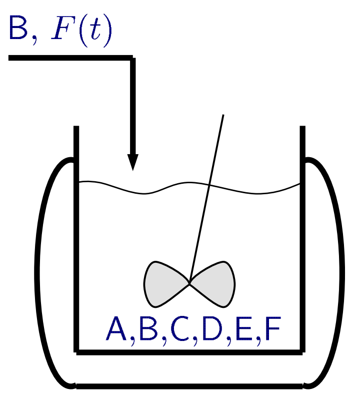
Run-to-Run Optimization of Semi-Batch Reactor

- **Industrial Reaction System**

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

Simulated Reality

Model



- Manipulated Variables: $F(t)$ (feed flow rate of B)
- Objective: Maximize $n_{\mathsf{C}}(t_f)$ (production of C)
- Constraints:

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

$c_{\mathsf{D}}(t_f) \leq 0.15$ mol l^{-1} (max. by-product concentration)

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

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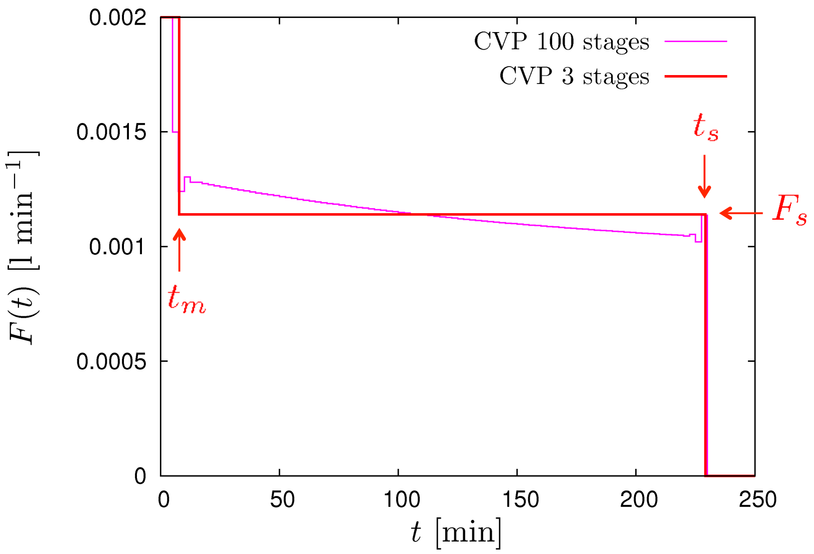
Nominal Input Trajectory



◦ **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

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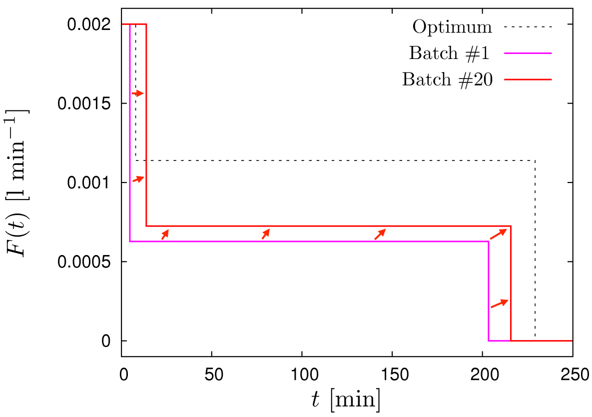
Adaptation of Model Parameters k_1 and k_2



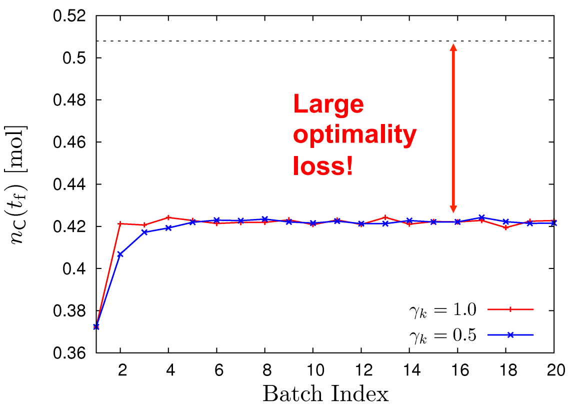
- **Measurement Noise:** $\sigma_y = 5\%$
  (10% constraint backoffs)

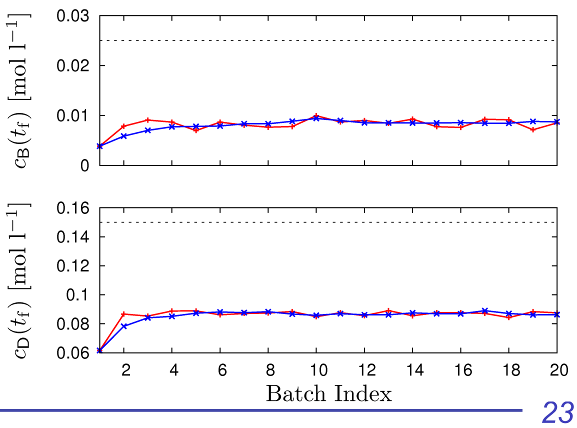
- **Identification Objective:**

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

- **Exponential Filter for k_1, k_2:**

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





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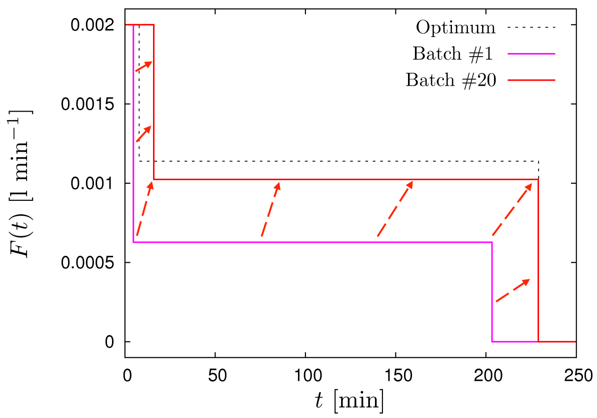
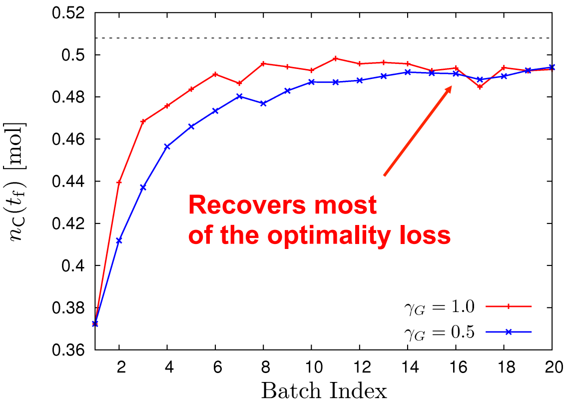
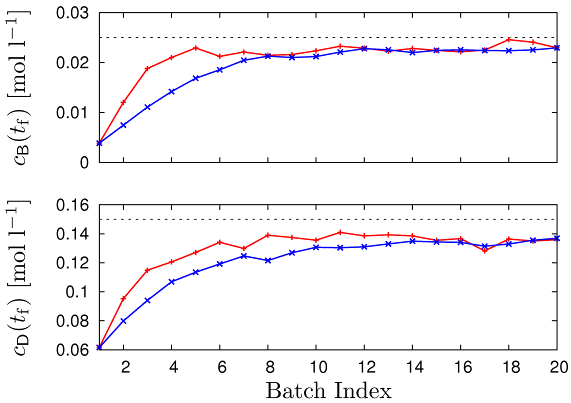
Adaptation of Modifiers ε_G



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

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





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Adaptation of Input Parameters t_s and F_s

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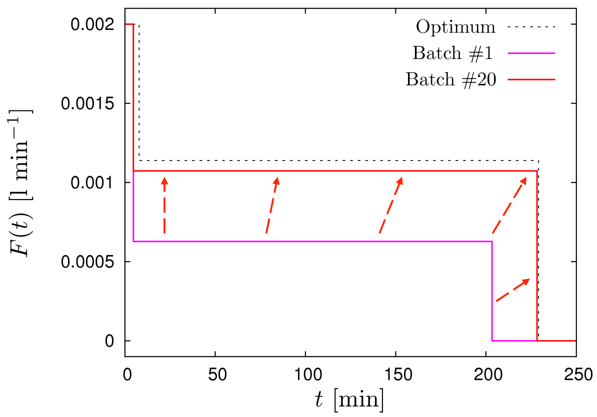
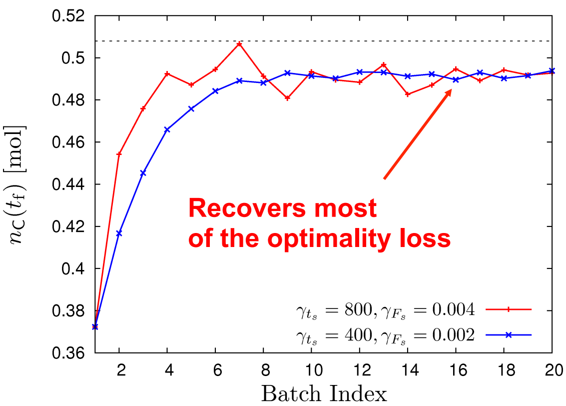
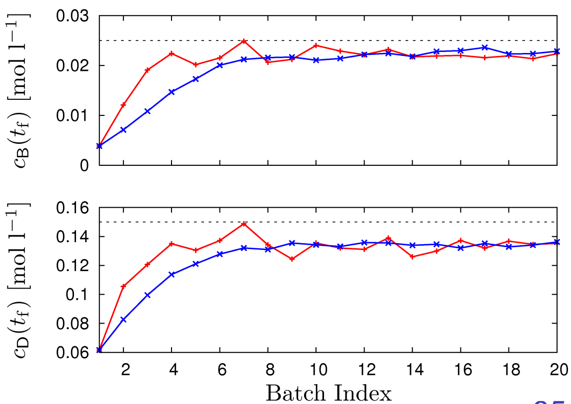


- **Measurement Noise:** $\sigma_y = 5\%$
  (10% constraint back-offs)
- **No Gradient Correction**
- **Controller Design:**

$t_m = 4.71$ min (fixed)

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





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Industrial Application of NCO Tracking

Emulsion Copolymerization Process

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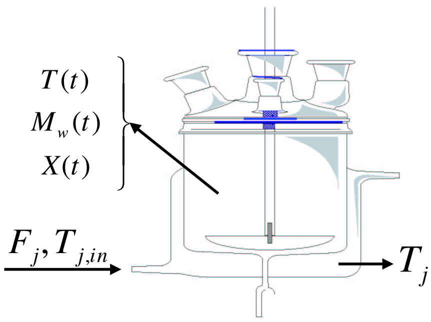
- Industrial features
  - 1-ton reactor, risk of runaway
  - Initiator efficiency can vary considerably
  - Several recipes
    - *different initial conditions*
    - *different initiator feeding policies*
    - *use of chain transfer agent*



- Modeling difficulties
- Uncertainty

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

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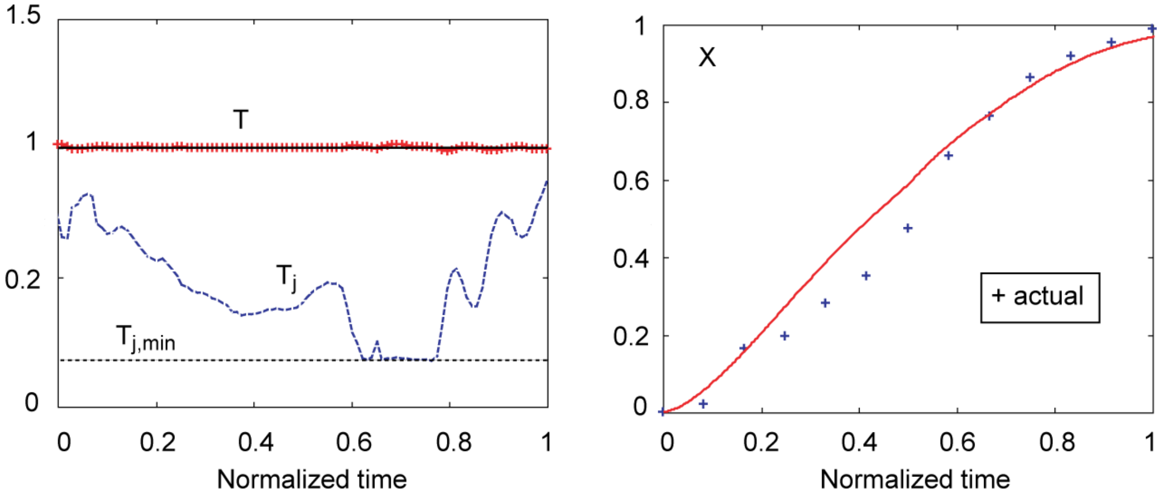
Industrial Practice



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Optimal Temperature Profile

Numerical Solution using a Tendency Model

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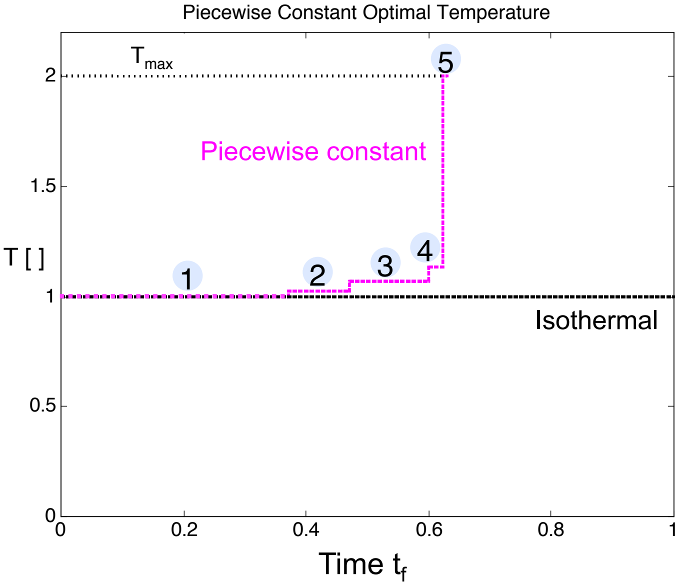

- Current practice: isothermal
- Numerical optimization
  - ✓ Piecewise-constant input
  - ✓ 5 decision variables (T_2-T_5, t_f)
  - ✓ Fixed relative switching times
- Active constraints
  - ✓ Interval 1: heat removal
  - ✓ Interval 5: T_{max}

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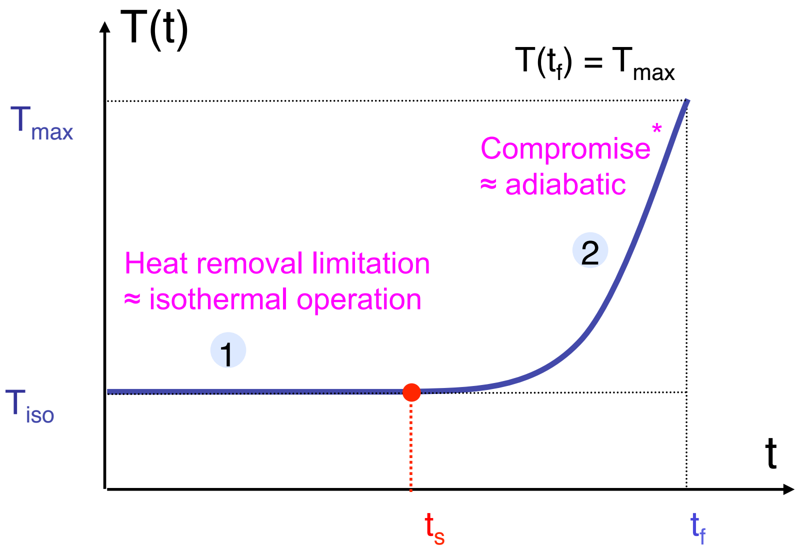
Model of the Solution -- Semi-adiabatic Profile



*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

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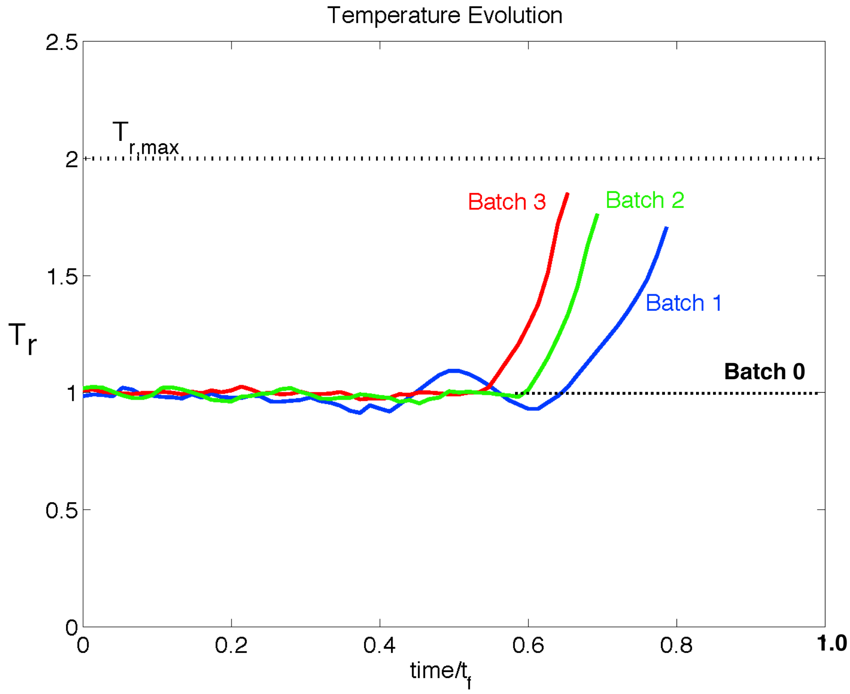
Industrial Results (1-ton reactor)



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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

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Conclusions

- How to use the measurements?
  - what are the best handles for correction?
- Repeated estimation and optimization has problems
  - model adequacy for optimization
- Practical observations
  - complexity depends on the number of inputs (not system order)
  - the solution is often determined by the constraints of the problem

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