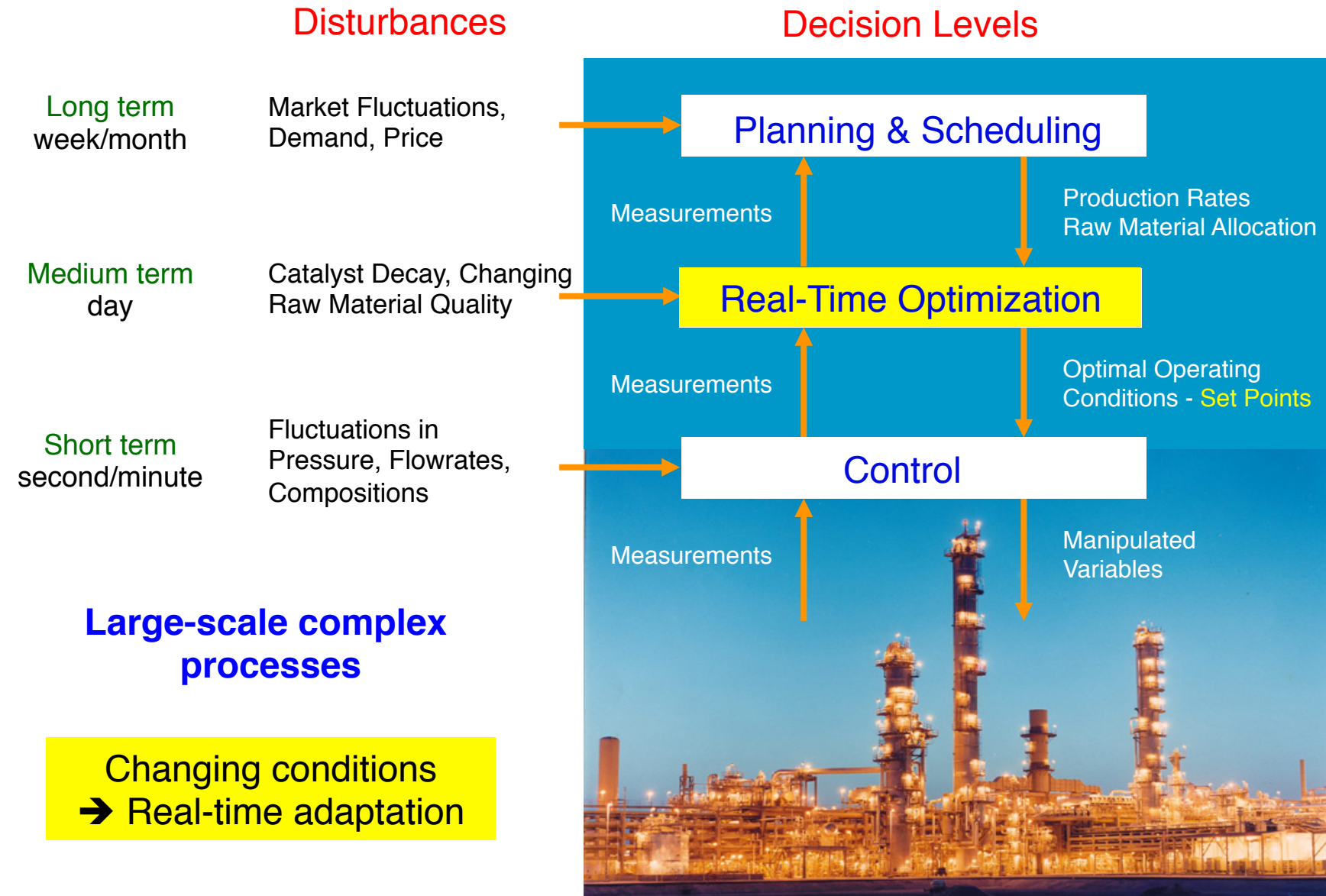


Real-Time Optimization of Chemical Processes

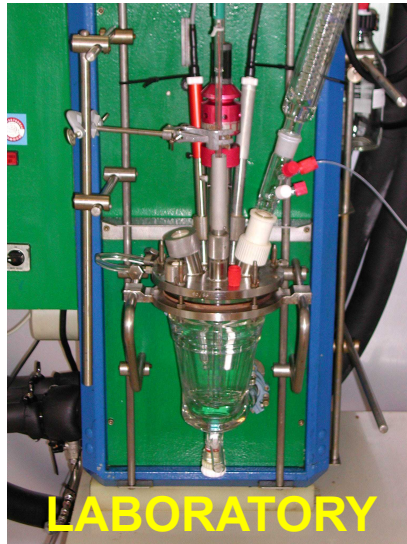
Dominique Bonvin, Grégory François and Gene Bunin
Laboratoire d'Automatique
EPFL, Lausanne

SFGP, Lyon 2013

Real-Time Optimization of a Continuous Plant

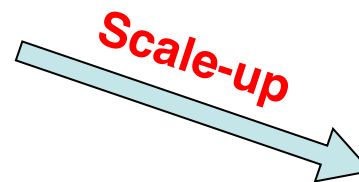


Optimization of a Discontinuous Plant



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

Outline

What is real-time optimization

- **Goal:** Optimal plant operation
- **Tool:** Model-based numerical optimization, experimental optimization
- Key feature: **use of real-time measurements**

Real-time optimization framework

- Three approaches
- Key issues: **Which measurements? How to best exploit them?**
- Simulated comparison

Experimental case studies

- Fuel-cell stack
- Batch polymerization

Static Optimization Problem

Optimize the steady-state **performance** of a (dynamic) process while satisfying a number of operating **constraints**

Plant

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

Optimal plant operation

Inputs \mathbf{u} ?
(set points)



Plant
Outputs \mathbf{y}_p

Model-based Optimization

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

NLP

Model-based numerical optimization

Model
Parameters $\boldsymbol{\theta}$?

Inputs \mathbf{u} ?
(set points)



Predicted
Outputs \mathbf{y}

Dynamic Optimization Problem

Optimize the dynamic **performance** of a (dynamic) process while satisfying a number of operating **constraints**

Plant

$$\begin{aligned} \min_{\mathbf{u}[0,t_f]} \quad & \Phi := \phi(\mathbf{x}_p(t_f)) \\ \text{s. t.} \quad & \mathbf{S}(\mathbf{x}_p, \mathbf{u}) \leq \mathbf{0} \\ & \mathbf{T}(\mathbf{x}_p(t_f)) \leq \mathbf{0} \end{aligned}$$

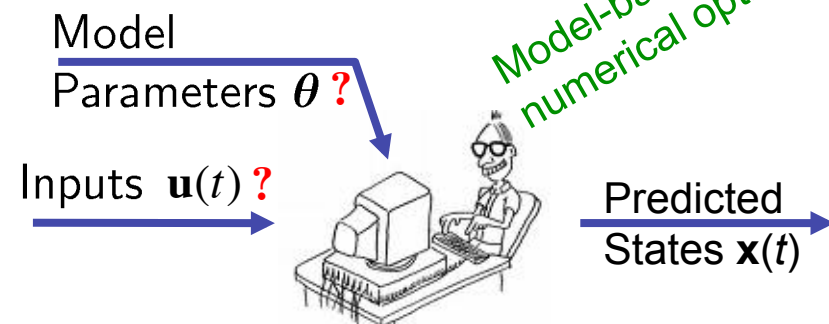
Optimal plant operation



Model-based Optimization

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

Model-based numerical optimization



Run-to-Run Optimization of a Batch Plant

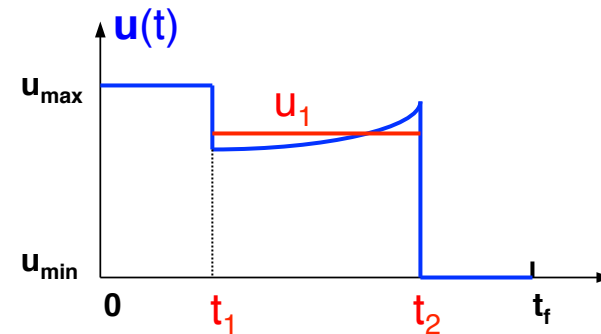


Batch plant with
finite terminal time

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

Input Parameterization

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



Batch plant
viewed as a static map

$$\begin{aligned} \min_{\boldsymbol{\pi}} \quad & \Phi(\boldsymbol{\pi}, \boldsymbol{\theta}) \\ \text{s. t.} \quad & \mathbf{G}(\boldsymbol{\pi}, \boldsymbol{\theta}) \leq \mathbf{0} \end{aligned}$$

NLP

Outline

What is real-time optimization

- Goal: Optimal plant operation
- Tool: Model-based numerical optimization, experimental optimization
- Key feature: use of real-time measurements

Real-time optimization framework

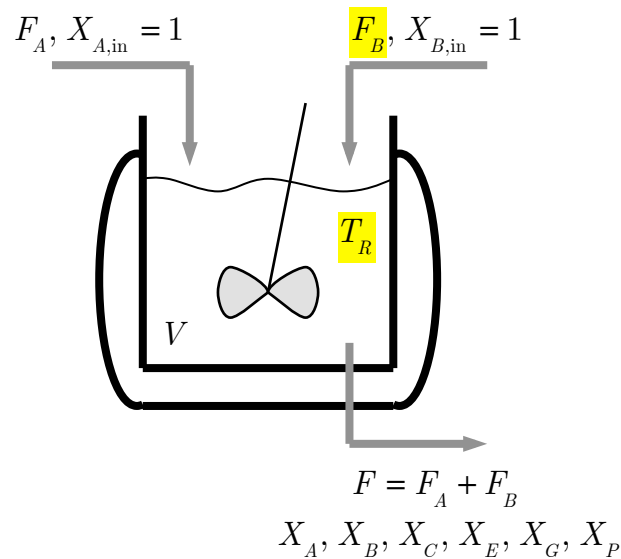
- Three approaches
- Key issues: **Which measurements? How to best exploit them?**
- Simulated comparison

Experimental case studies

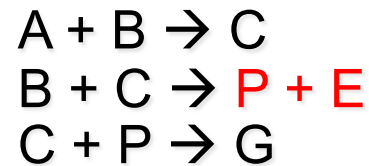
- Fuel-cell stack
- Batch polymerization

Example of Plant-Model Mismatch

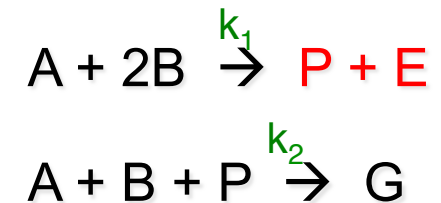
Williams-Otto reactor



3-reaction system



2-reaction model



Objective: maximize operating profit

Model

- 4th-order model
- 2 inputs
- 2 adjustable parameters (k_{10}, k_{20})

Three RTO Approaches

How to best exploit the measurements?

Optimization in the presence
of **Uncertainty**

No Measurement:
Robust Optimization

Measurements:
Adaptive Optimization

$$\mathbf{u}^* \in \arg \min_{\mathbf{u}} \phi(\mathbf{u}, \mathbf{y})$$

s.t. $\mathbf{F}(\mathbf{u}, \mathbf{y}, \boldsymbol{\theta}) = \mathbf{0}$
 $\mathbf{g}(\mathbf{u}, \mathbf{y}) \leq \mathbf{0}$

input update: $\delta \mathbf{u}$
 parameter update: $\delta \boldsymbol{\theta}$
 cost & constraint update: $\delta \mathbf{g}, \delta \phi$

Adaptation of
Model Parameters

- two-step approach
(repeated identification
and optimization)

Adaptation of
Cost & Constraints

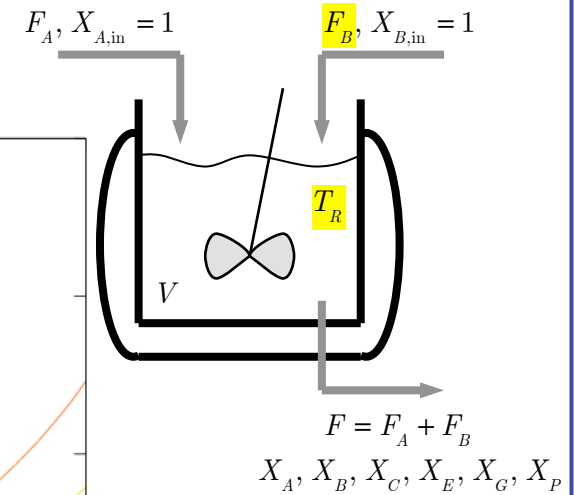
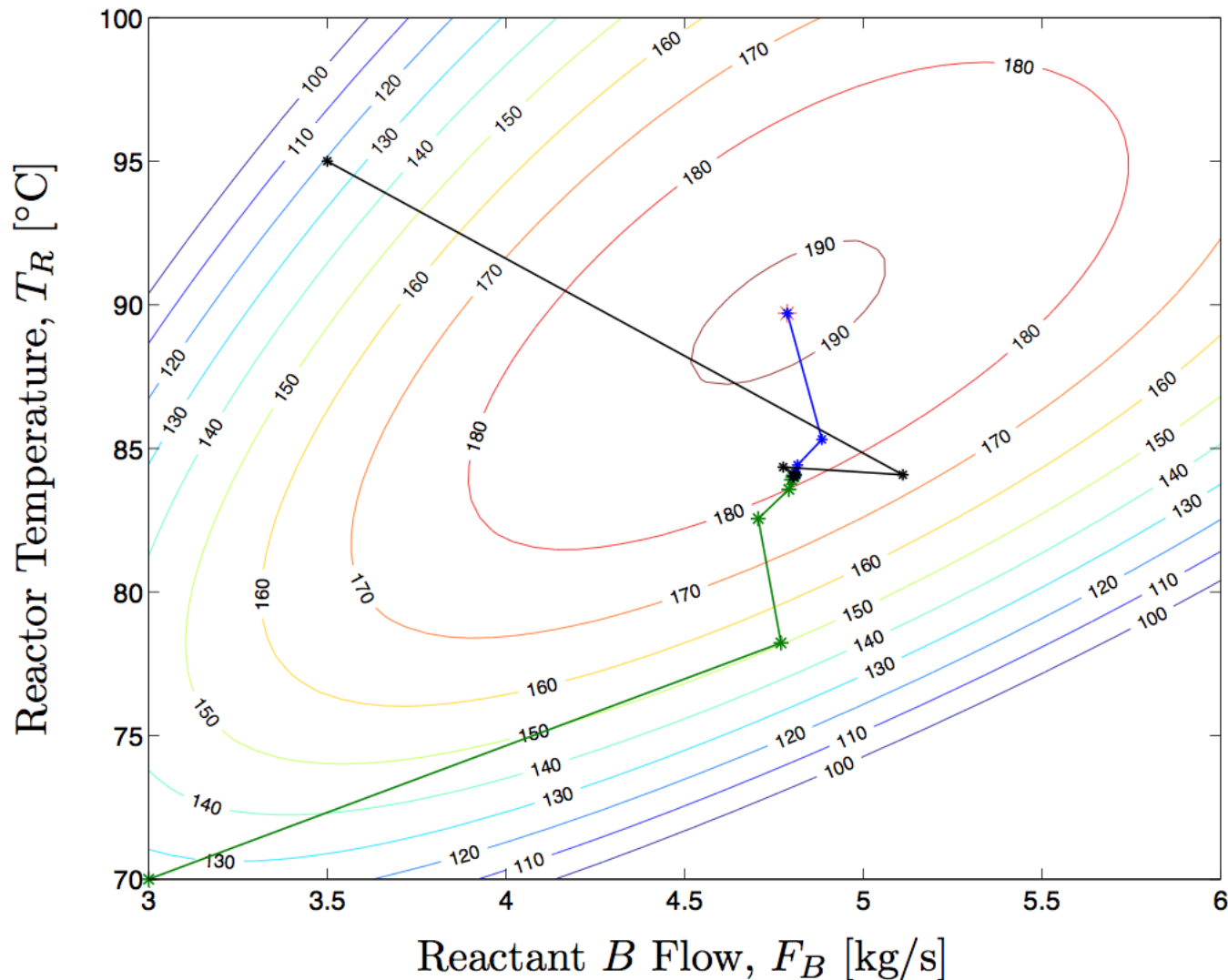
- bias update
- constraint update
- gradient correction
- modifier adaptation

Adaptation of
Inputs

- tracking active constraints
- NCO tracking
- extremum-seeking control
- self-optimizing control

1. Adaptation of Model Parameters

Two-step approach



Williams-Otto Reactor

- 4th-order model
- 2 inputs
- 2 adjustable par.

Does not
converge to plant
optimum

Two-step approach

Parameter Estimation Problem

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

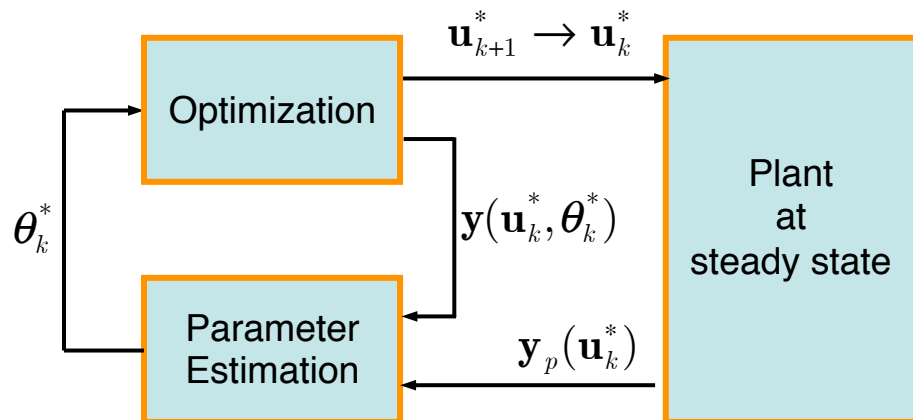
$$J_k^{\text{id}} = \left[\mathbf{y}_p(\mathbf{u}_k^*) - \mathbf{y}(\mathbf{u}_k^*, \theta) \right]^T \mathbf{Q} \left[\mathbf{y}_p(\mathbf{u}_k^*) - \mathbf{y}(\mathbf{u}_k^*, \theta) \right]$$

Optimization Problem

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

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

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

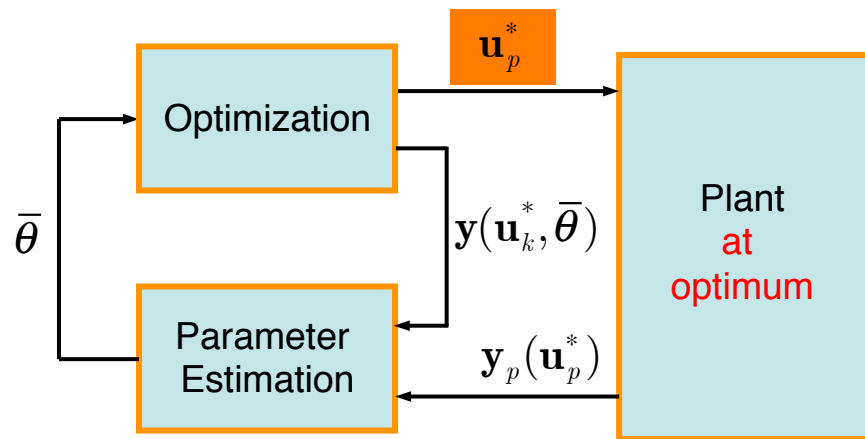


Current Industrial Practice
for tracking the changing optimum
in the presence of disturbances

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

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

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

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

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

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

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

SOSC

Par.
Est.

Opt.

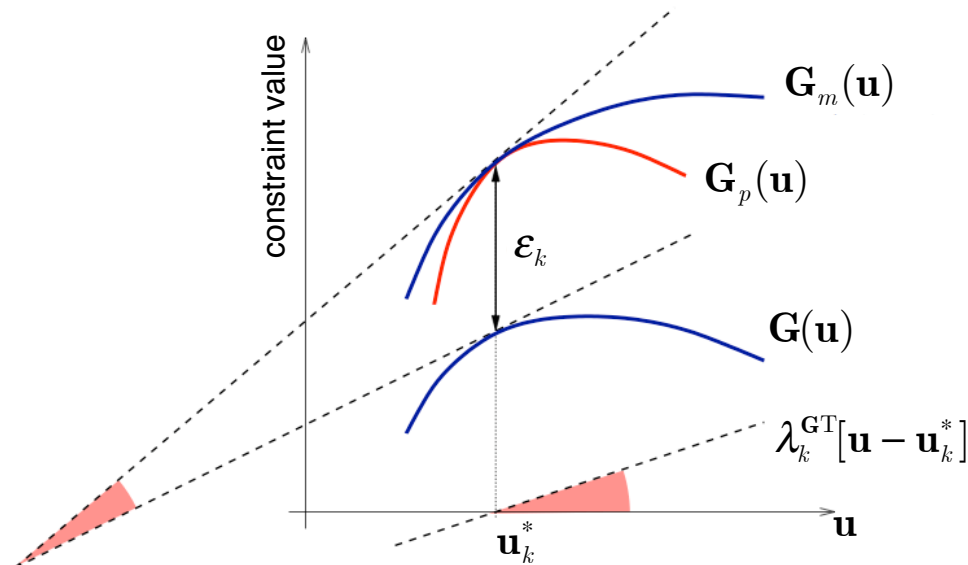
J.F. Forbes, T.E. Marlin. Design Cost: A Systematic Approach to Technology Selection for Model-Based Real-Time Optimization Systems. *Comp. Chem. Eng.*, **20**(6/7), 717-734, 1996

2. Adaptation of Cost & Constraints Input-Affine Correction to the Model

Modified Optimization Problem

$$\begin{aligned} \mathbf{u}_{k+1}^* \in \arg \min_{\mathbf{u}} \quad & \Phi_m(\mathbf{u}) := \Phi(\mathbf{u}) + \lambda_k^{\Phi T} [\mathbf{u} - \mathbf{u}_k^*] \\ \text{s.t.} \quad & \mathbf{G}_m(\mathbf{u}) := \mathbf{G}(\mathbf{u}) + \varepsilon_k + \lambda_k^{\mathbf{G} T} [\mathbf{u} - \mathbf{u}_k^*] \leq 0 \\ & \mathbf{u}^L \leq \mathbf{u} \leq \mathbf{u}^U \end{aligned}$$

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

Input-Affine Correction to the Model

Modified Optimization Problem

$$\begin{aligned} \mathbf{u}_{k+1}^* \in \arg \min_{\mathbf{u}} \quad & \Phi_m(\mathbf{u}) := \Phi(\mathbf{u}) + \lambda_k^{\Phi^T} [\mathbf{u} - \mathbf{u}_k^*] \\ \text{s.t.} \quad & \mathbf{G}_m(\mathbf{u}) := \mathbf{G}(\mathbf{u}) + \boldsymbol{\varepsilon}_k + \lambda_k^{\mathbf{G}^T} [\mathbf{u} - \mathbf{u}_k^*] \leq \mathbf{0} \\ & \mathbf{u}^L \leq \mathbf{u} \leq \mathbf{u}^U \end{aligned}$$

- KKT Elements: $\mathbf{c}^T = \left(G_1, \dots, G_{n_g}, \frac{\partial G_1}{\partial \mathbf{u}}, \dots, \frac{\partial G_{n_g}}{\partial \mathbf{u}}, \frac{\partial \Phi}{\partial \mathbf{u}} \right) \in \mathbb{R}^{n_K} \quad n_K = n_g + n_u(n_g + 1)$
- KKT Modifiers: $\Lambda^T = \left(\boldsymbol{\varepsilon}_1, \dots, \boldsymbol{\varepsilon}_{n_g}, \lambda^{G_1^T}, \dots, \lambda^{G_{n_g}^T}, \lambda^{\Phi^T} \right) \in \mathbb{R}^{n_K}$

Modifier Adaptation (without filter)

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

Requires evaluation of
KKT elements of plant

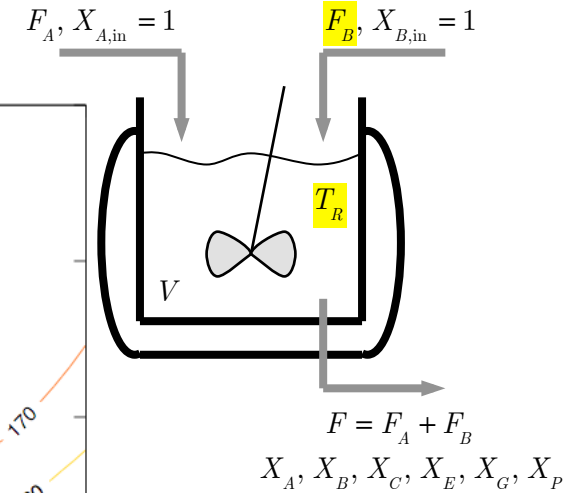
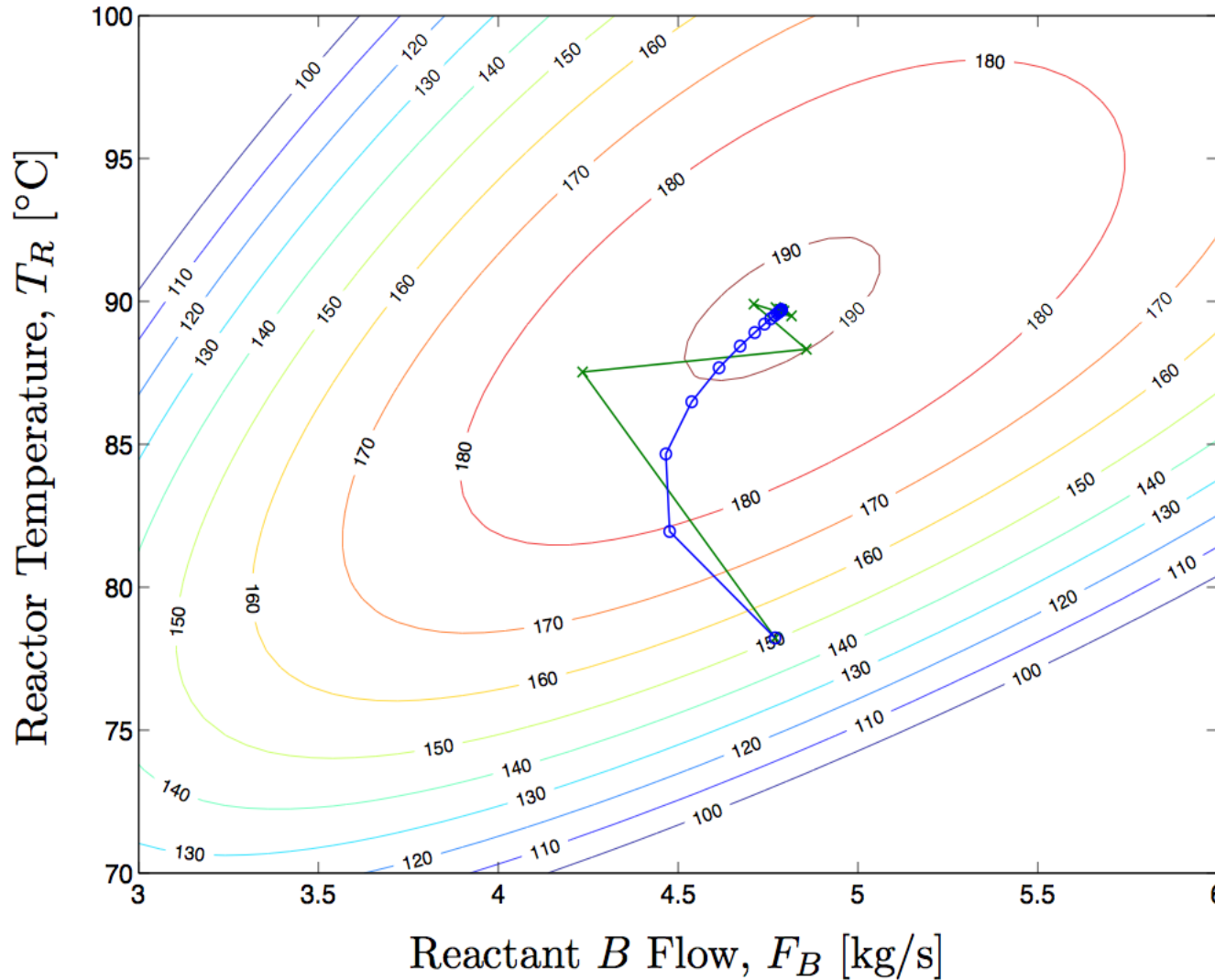
Modifier Adaptation (with filter)

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

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)

Example Revisited

Modifier adaptation



Williams-Otto Reactor

- 4th-order model
- 2 inputs
- 2 adjustable par.

Converges to plant optimum

Modeling for Optimization

Features of a “good” model

- Must be able to predict the optimality conditions of the plant:
active constraints and (reduced) gradients
- Focuses on the optimal solution
→ **“solution model”** rather than “plant model”

Need to be able to estimate the plant gradients

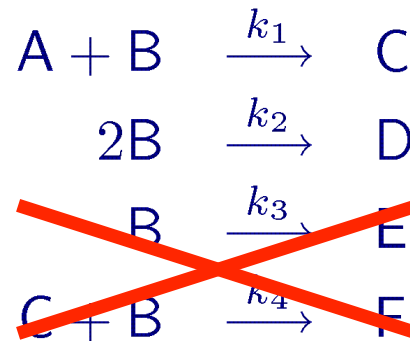
- From cost and constraint values at previous operating points
- Must be able to use the key measurements (active constraints and gradients)

Run-to-Run Optimization of Semi-Batch Reactor

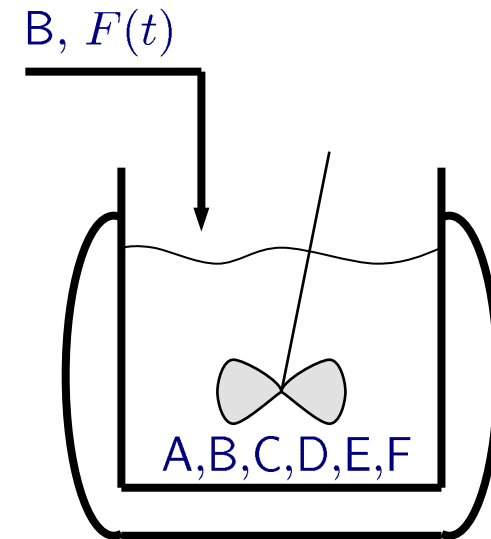
- Industrial Reaction System

Lonza

*Simulated
Reality*



Model



- Manipulated Variables: $F(t)$ (feed flow rate of B)

- Objective: **Maximize** $n_C(t_f)$ (production of C)

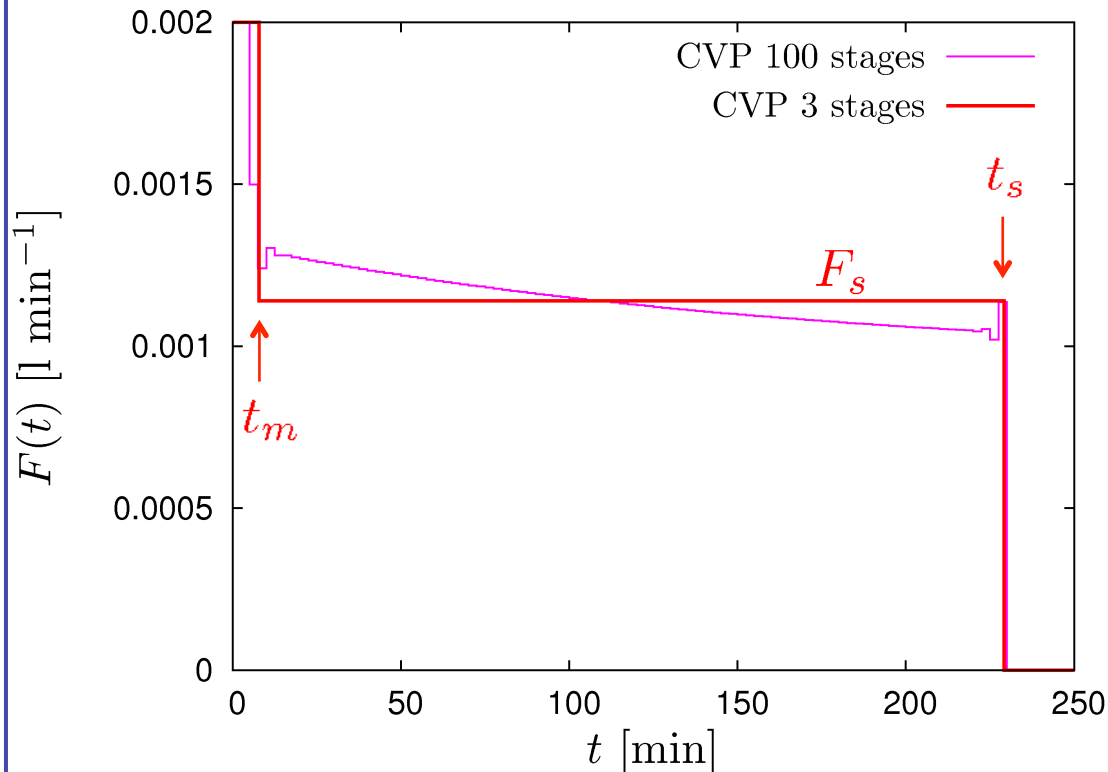
- Constraints:

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 Optimal Input



Plant model

- 3 nonlinear balance equations
- 2 uncertain parameters k_1 and k_2
- Measurements to adjust k_1 and k_2

A solution model

- 3 arcs: F_{\max} , F_s and F_{\min}
- 3 adjustable parameters t_m , t_s and F_s
- Measurements to adjust t_m , t_s and F_s

○ Optimal Solution

3 arcs, 2 active terminal constraints

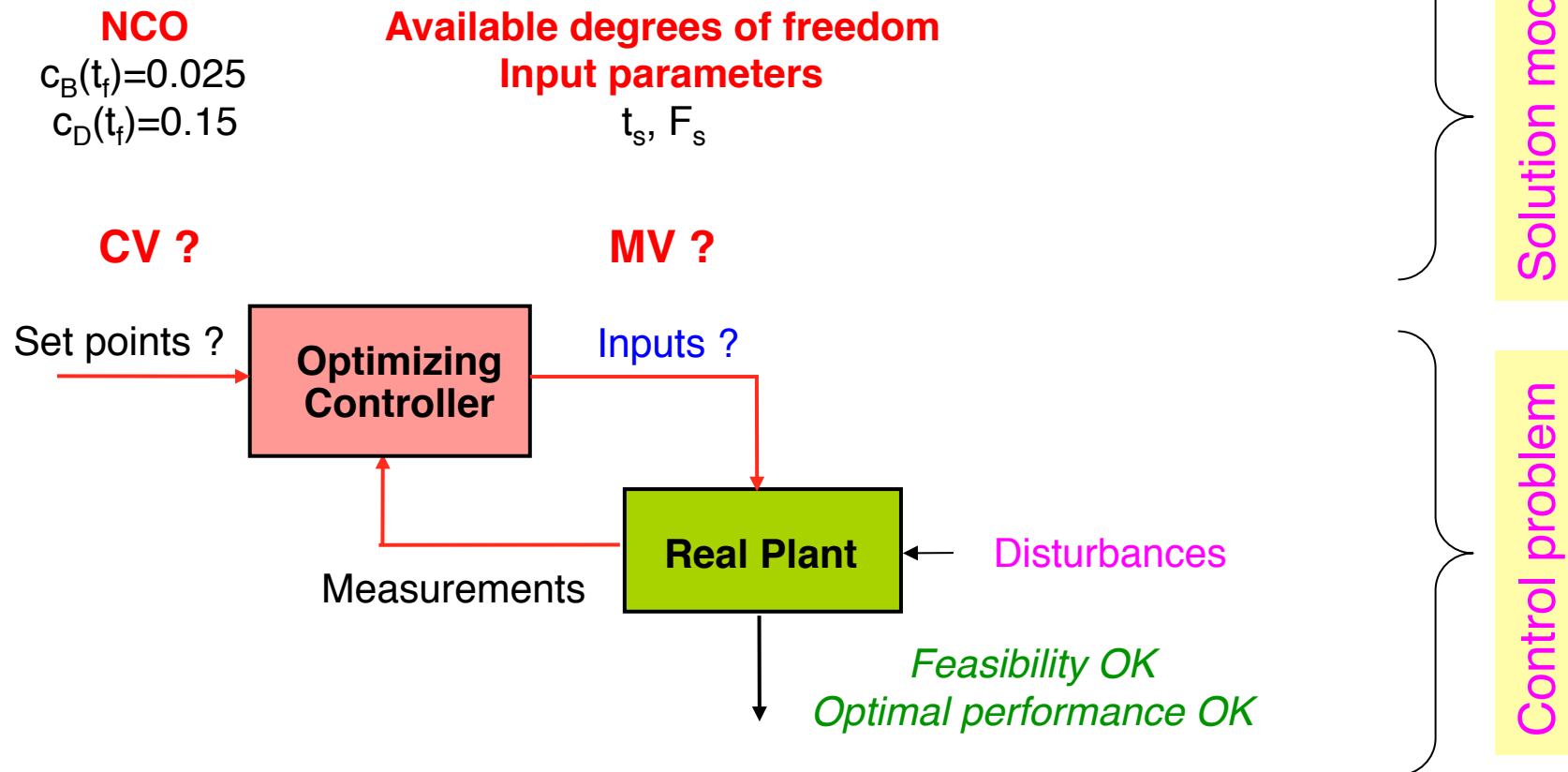
$$J^* \approx 0.5081 \text{ mol}$$

○ Approximate Solution

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

$$J^* \approx 0.5079 \text{ mol}$$

3. Adaptation of Inputs NCO tracking



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

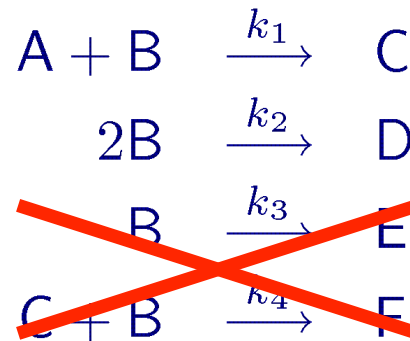
Comparison of RTO Schemes

Run-to-Run Optimization of Semi-Batch Reactor

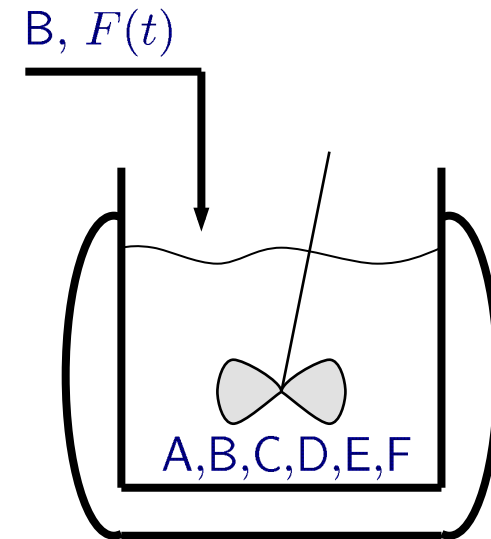
- Industrial Reaction System

Lonza

*Simulated
Reality*



Model



- Manipulated Variables: $F(t)$ (feed flow rate of B)

- Objective: **Maximize** $n_C(t_f)$ (production of C)

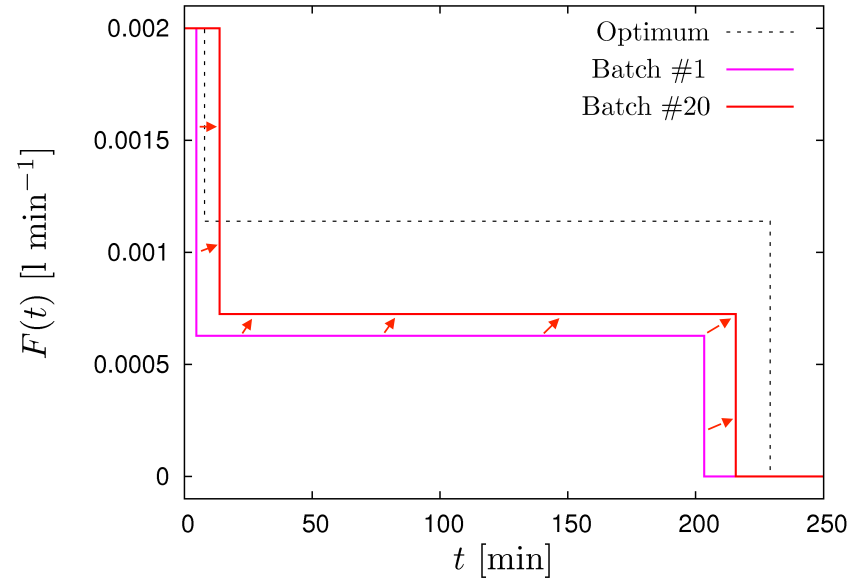
- Constraints:

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

Adaptation of Model Parameters k_1 and k_2



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

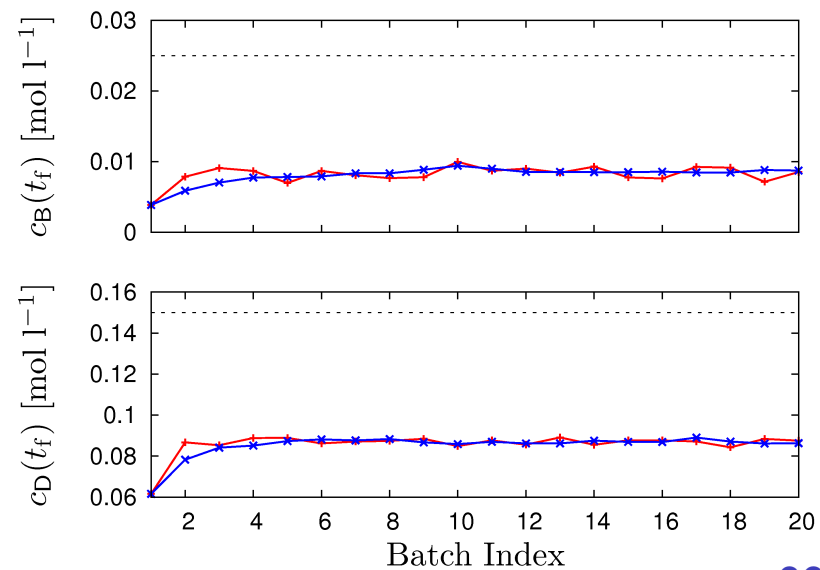
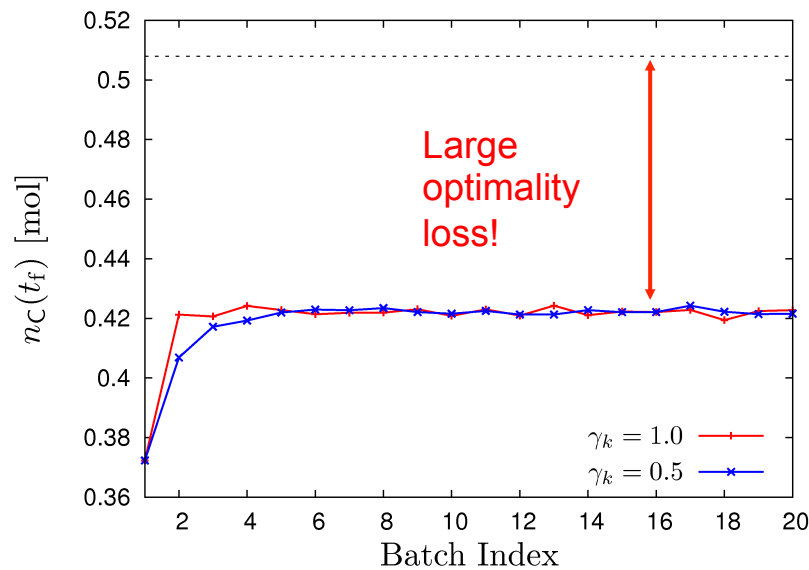
- Identification Objective:

$$J^{id} = \sum_{k=1}^{n^{meas}} \left[\frac{y - y^{meas}}{\bar{y}} \right]_{t=t_k}^2, \quad y = (c_B, c_C, c_D)$$

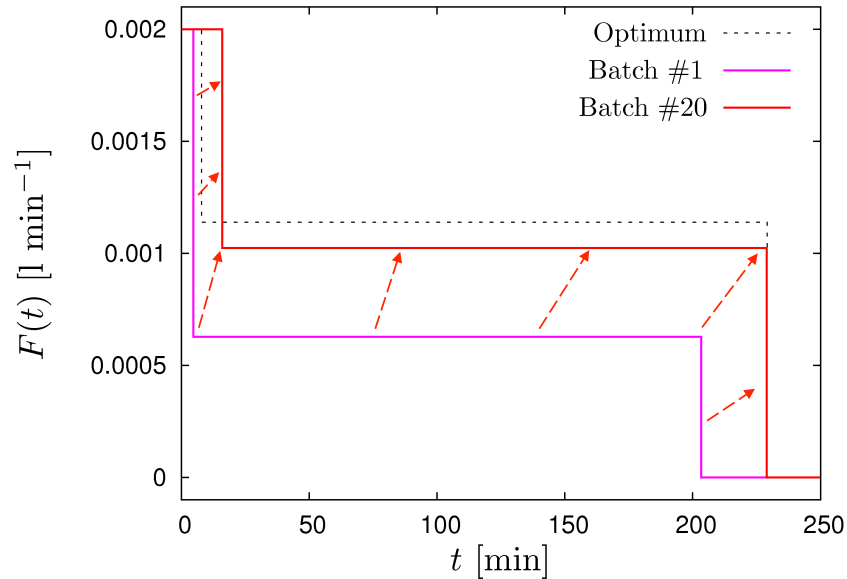
$n^{meas} = 6$

- Exponential Filter for k_1, k_2 :

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



Adaptation of Constraint Modifiers ε_G

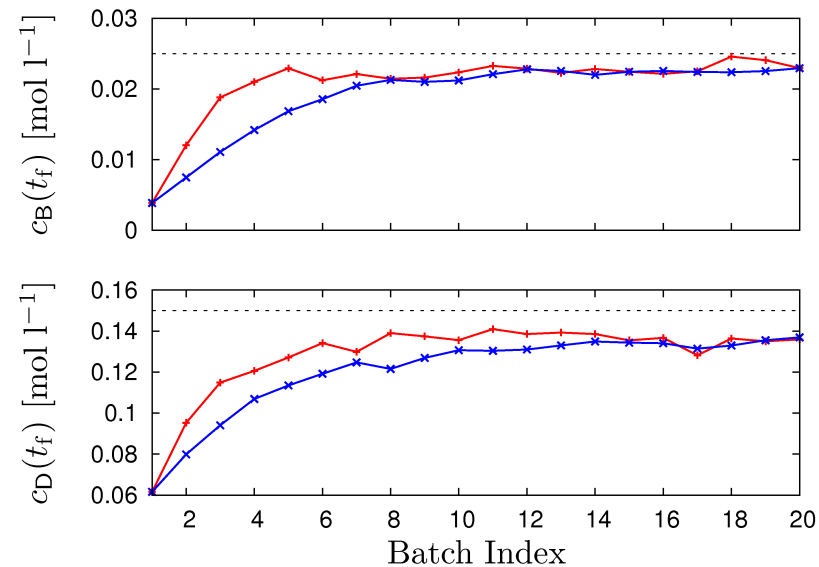
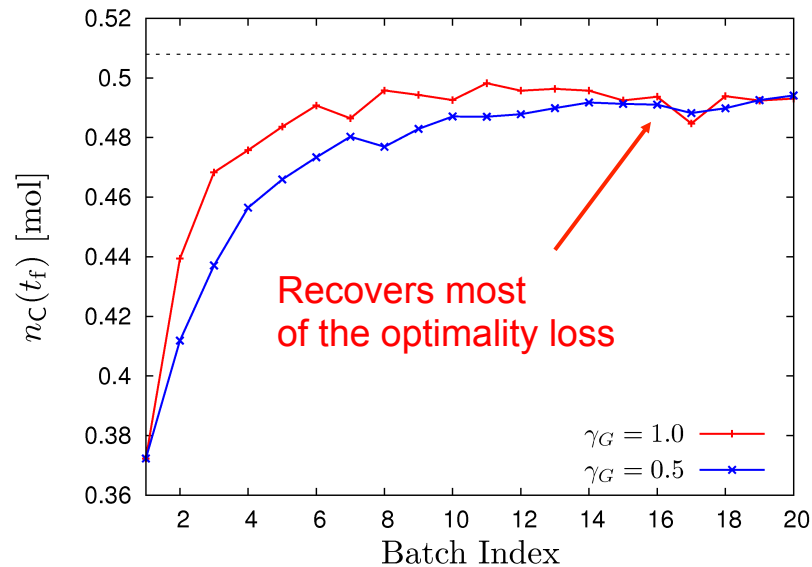


- Measurement Noise: $\sigma_y = 5\%$
(10% constraint backoffs)

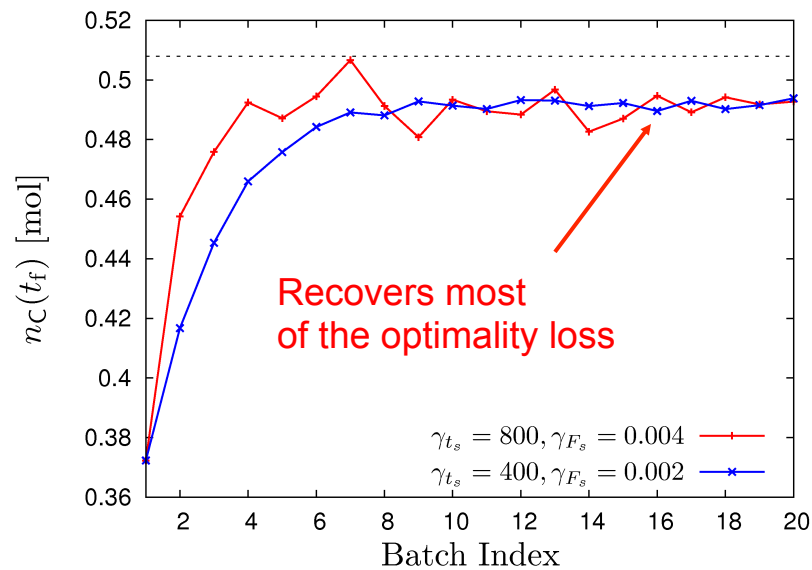
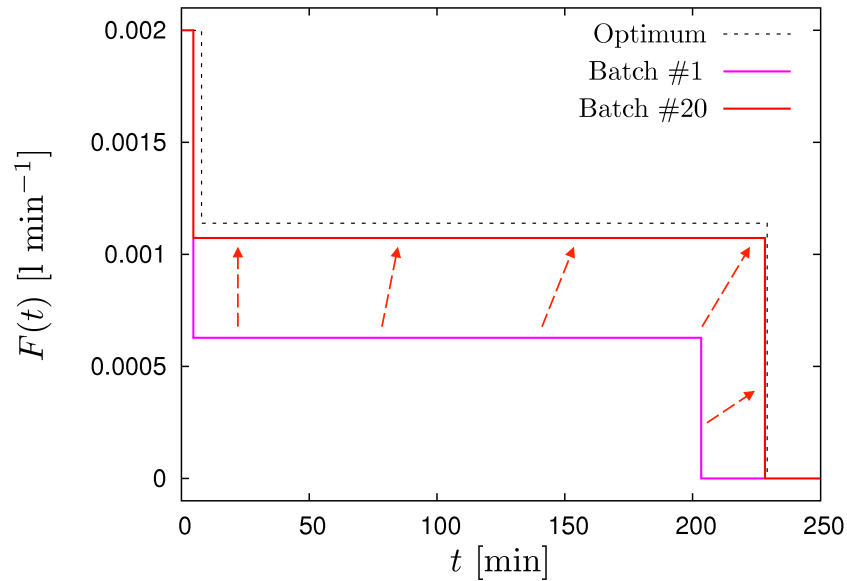
No Gradient Correction

- Exponential Filter for Modifiers:

$$\begin{pmatrix} \varepsilon_{G,1}^i \\ \varepsilon_{G,2}^i \end{pmatrix} = (1 - \gamma_G) \begin{pmatrix} \varepsilon_{G,1}^{i-1} \\ \varepsilon_{G,2}^{i-1} \end{pmatrix} + \gamma_G \begin{pmatrix} c_B^{\text{meas}}(t_f) - c_B(t_f) \\ c_D^{\text{meas}}(t_f) - c_D(t_f) \end{pmatrix}_{\pi = \pi^{i-1}}$$



Adaptation of Input Parameters t_s and F_s



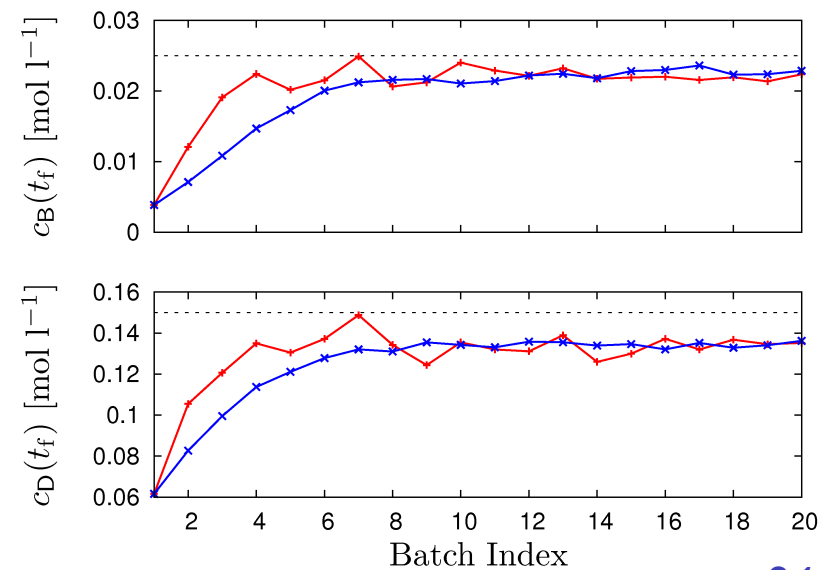
- Measurement Noise: $\sigma_y = 5\%$
(10% constraint back-offs)

- No Gradient Correction

- Controller Design:

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

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



Outline

What is real-time optimization

- Goal: Optimal plant operation
- Tool: Model-based numerical optimization, experimental optimization
- Key feature: use of real-time measurements

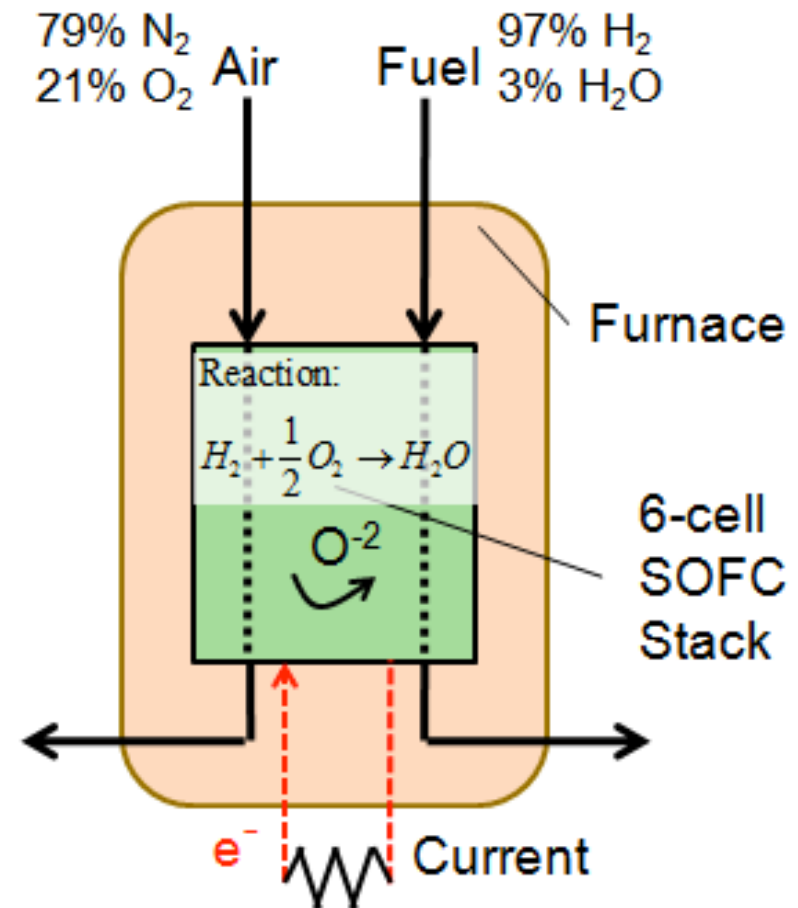
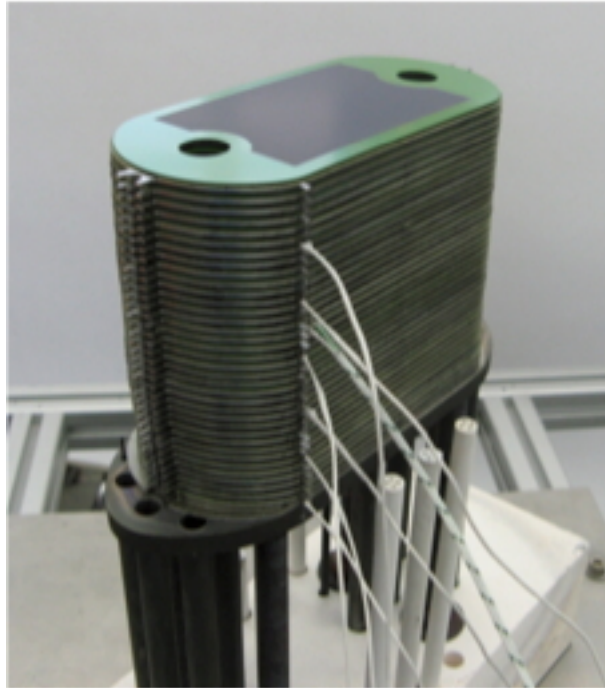
Real-time optimization framework

- Three approaches
- Key issues: Which measurements? How to best exploit them?
- Simulated comparison

Experimental case studies

- Fuel-cell stack
- Batch polymerization

Solid Oxide Fuel Cell Stack



- Stack of 6 cells, active area of 50 cm², metallic interconnector
- Anodes : standard nickel/yttrium stabilized-zirconia (Ni-YSZ)
- Electrolyte : dense YSZ.
- Cathodes: screen-printed (La, Sr)(Co, Fe)O₃
- Operation temperatures between 650 and 850°C.

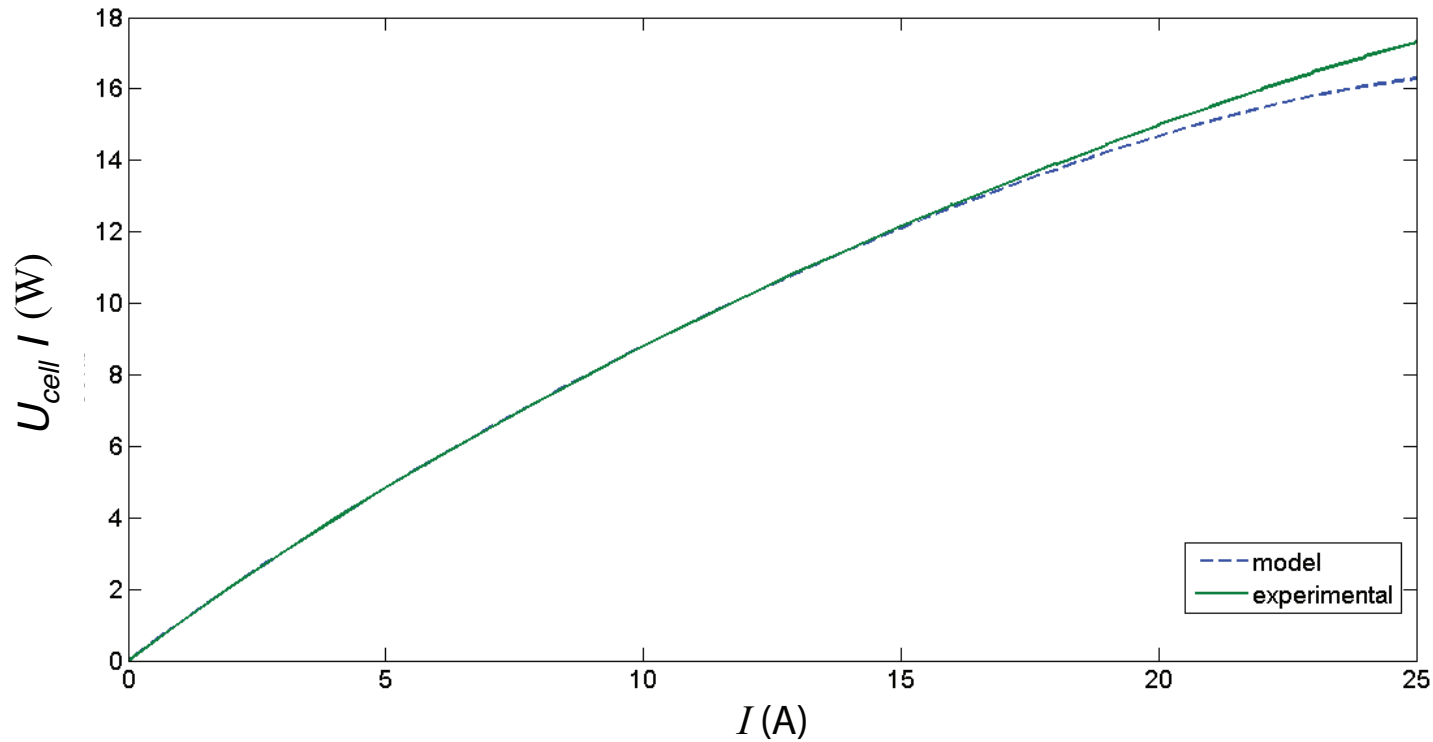
G.A. Bunin, Z. Wullemin, G. François, A. Nakajo, L. Tsikonis and D. Bonvin, Experimental real-time optimization of a solid oxide fuel cell stack via constraint adaptation, *Energy*, **39**(1), 54-62 (2012).

RTO via Constraint Adaptation

Experimental features

- Inputs: flowrates (H_2 , O_2), current (or load)
- Outputs: power density, cell potential, electrical efficiency
- Time-scale separation
 - *slow temperature dynamics, treated as process drift !*
 - *static model (for the rest)*
- Power demand changes without prior knowledge
- Inaccurate model in the operating region (power, cell)

RTO via Constraint Adaptation



Challenge: Implement optimal operation with changing power demand

RTO via Constraint Adaptation

Problem Formulation

At each RTO instant k , solve a static optimization problem, with a zeroth-order modifier in the constraints, **regardless of the fact that T has reached steady state or not**

$$\max_{u_k} \eta(\mathbf{u}_k, \Theta)$$

$$\text{s.t.} \quad p_{el}(\mathbf{u}_k, \Theta) + \varepsilon_{k-1}^{p_{el}} = p_{el}^S$$

$$U_{cell}(\mathbf{u}_k, \Theta) + \varepsilon_{k-1}^{U_{cell}} \geq 0.75V$$

$$v(\mathbf{u}_k) \leq 0.75$$

$$4 \leq 2 \frac{u_{2,k}}{u_{1,k}} = \lambda_{air}(\mathbf{u}_k) \leq 7$$

$$u_{1,k} \geq 3.14 \text{ mL}/(\text{min cm}^2)$$

$$u_{3,k} \leq 30A$$

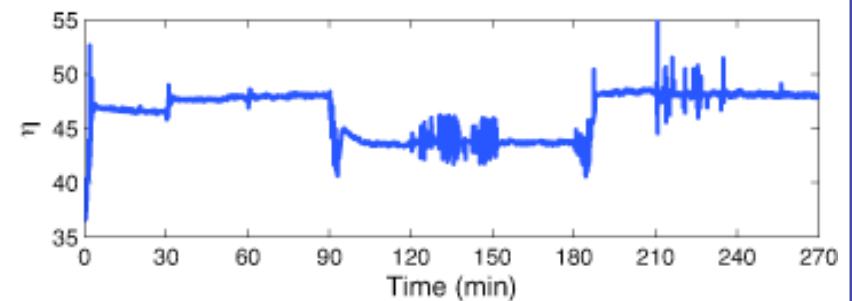
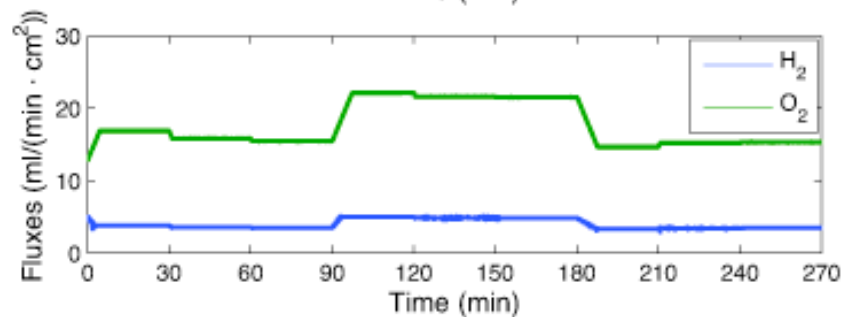
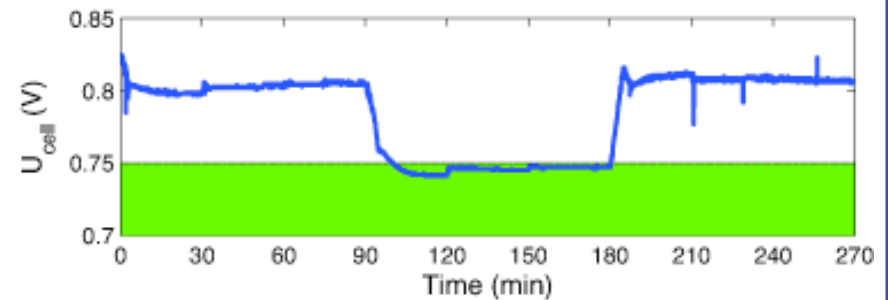
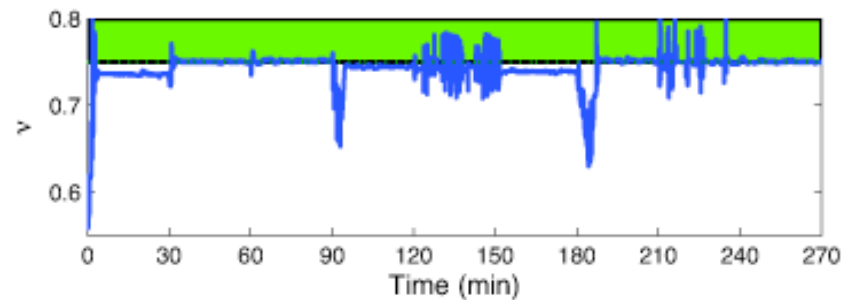
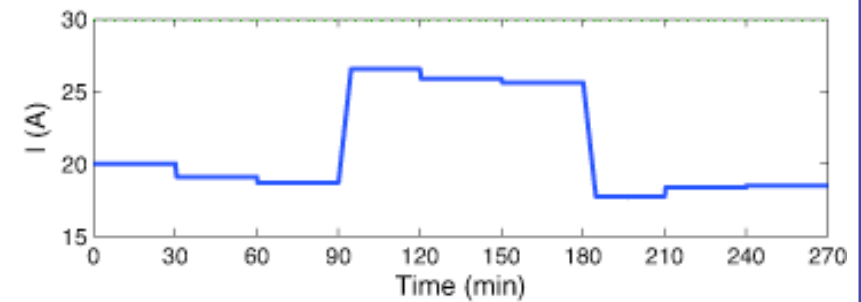
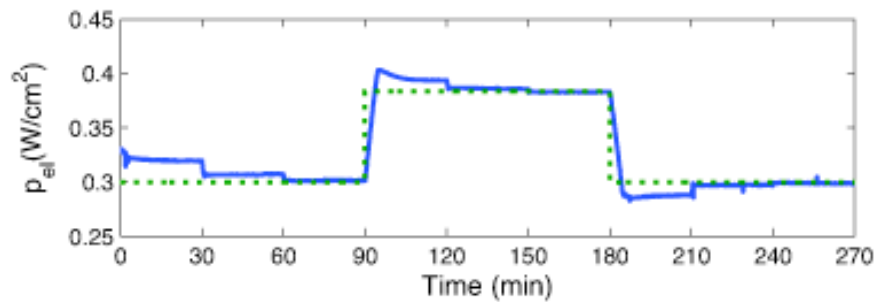
$$u_k = \begin{bmatrix} u_{1,k} = \dot{n}_{H_2,k} \\ u_{2,k} = \dot{n}_{O_2,k} \\ u_{3,k} = I_k \end{bmatrix}$$

$$\varepsilon_k^{p_{el}} = (1 - K_{p_{el}}) \varepsilon_{k-1}^{p_{el}} + K_{p_{el}} [p_{el,p,k} - p_{el}(\mathbf{u}_k, \Theta)]$$

$$\varepsilon_k^{U_{cell}} = (1 - K_{U_{cell}}) \varepsilon_{k-1}^{U_{cell}} + K_{U_{cell}} [U_{cell,p,k} - U_{cell}(\mathbf{u}_k, \Theta)]$$

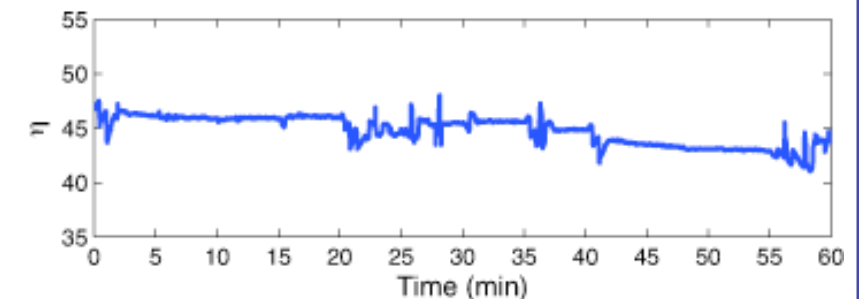
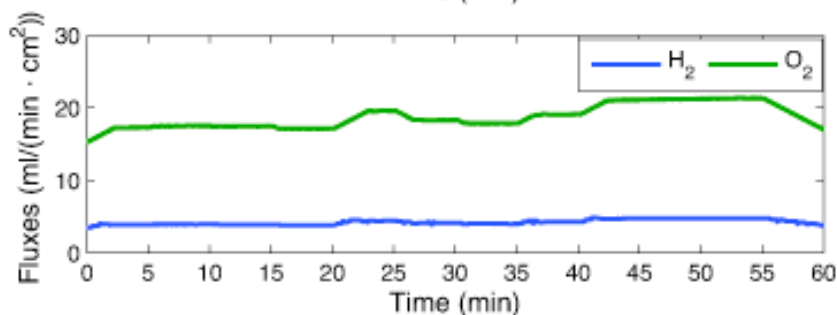
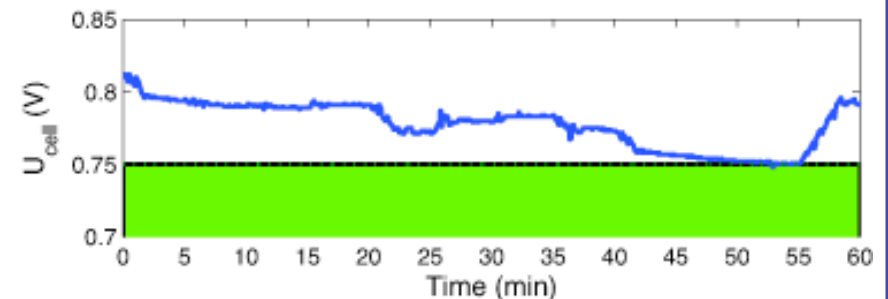
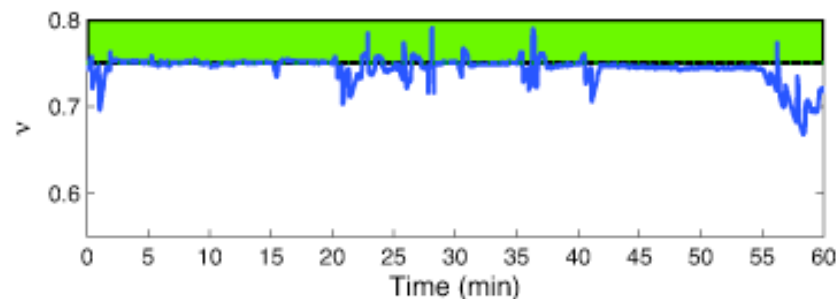
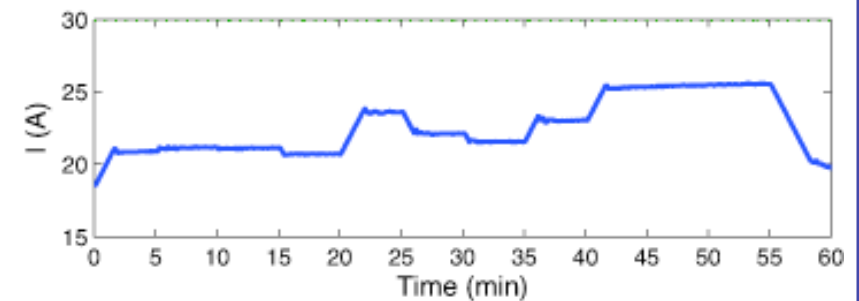
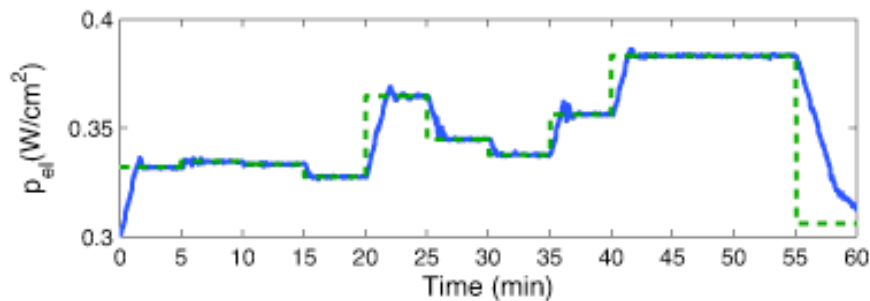
Slow RTO (“Wait for Steady State”)

- RTO very 30 min
- Unknown power changes every 90 min



Fast RTO with Random Power Changes

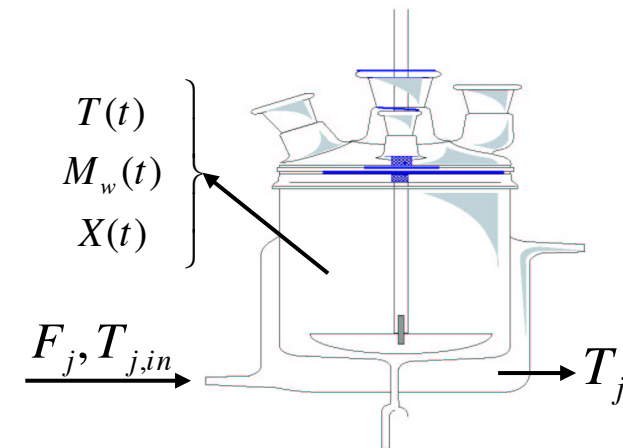
- Use steady-state model for predicting temperature
- RTO every 10 s, load changes every 5 min



Emulsion Copolymerization Process

Industrial process

- 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*

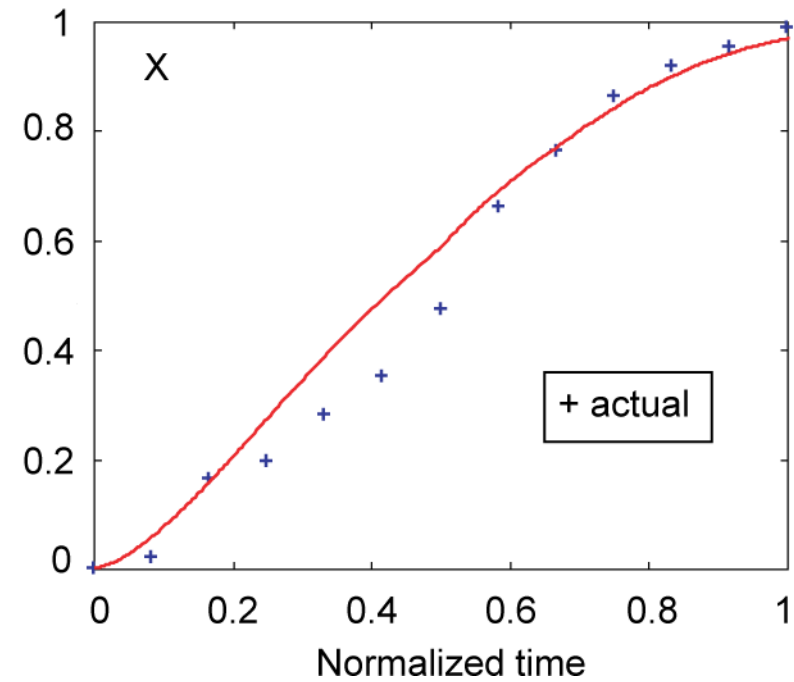
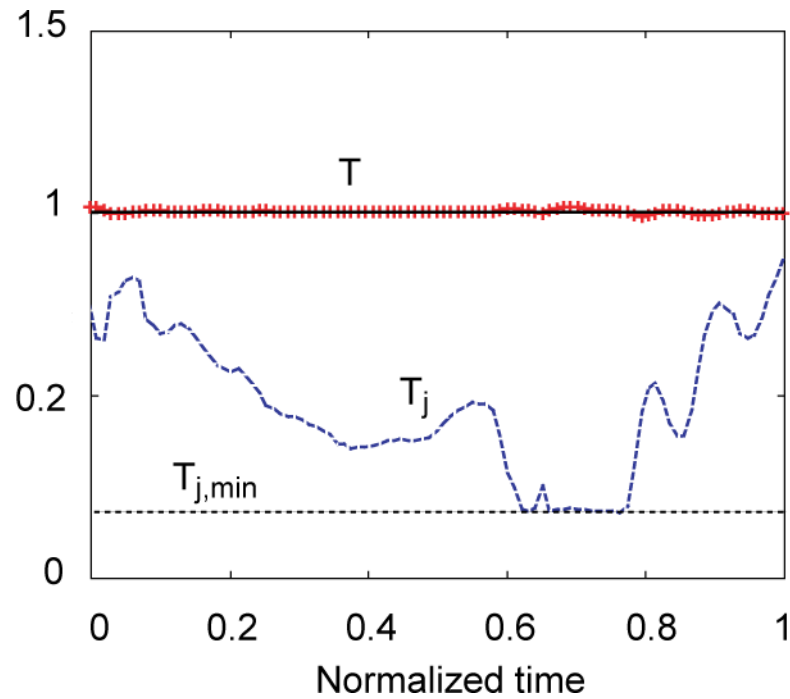


- Modeling difficulties
- Uncertainty

Objective: Minimize **batch time** by adjusting the reactor temperature

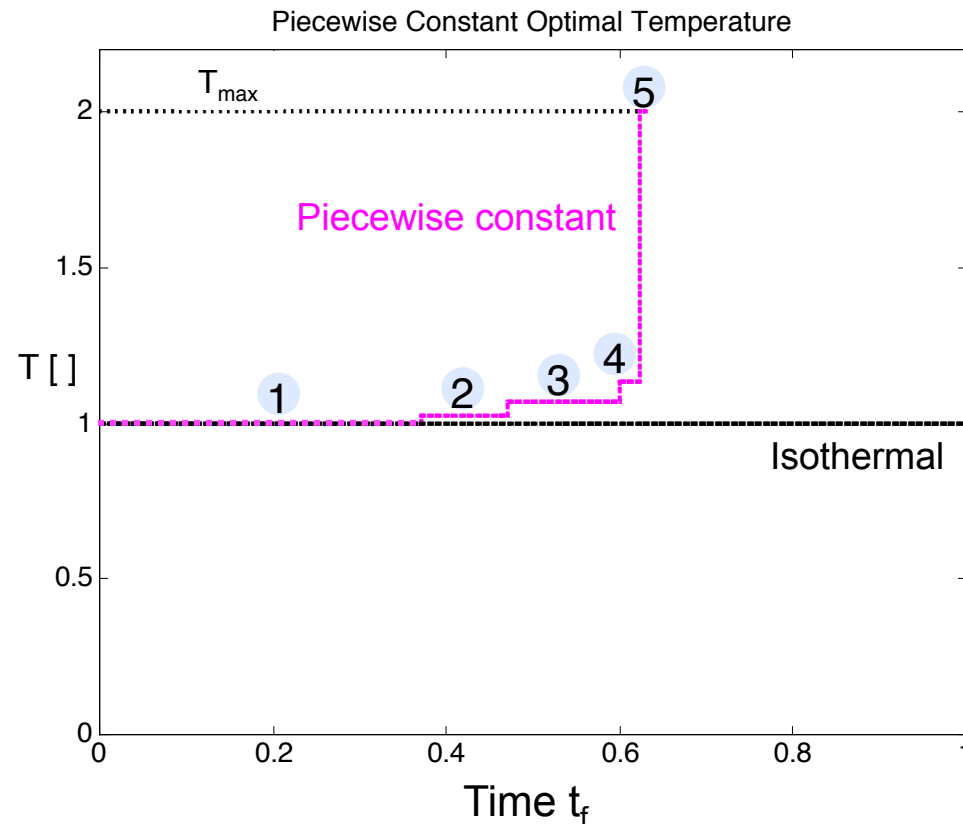
- Temperature and heat removal constraints
- Quality constraints at final time

Industrial Practice



Optimal Temperature Profile

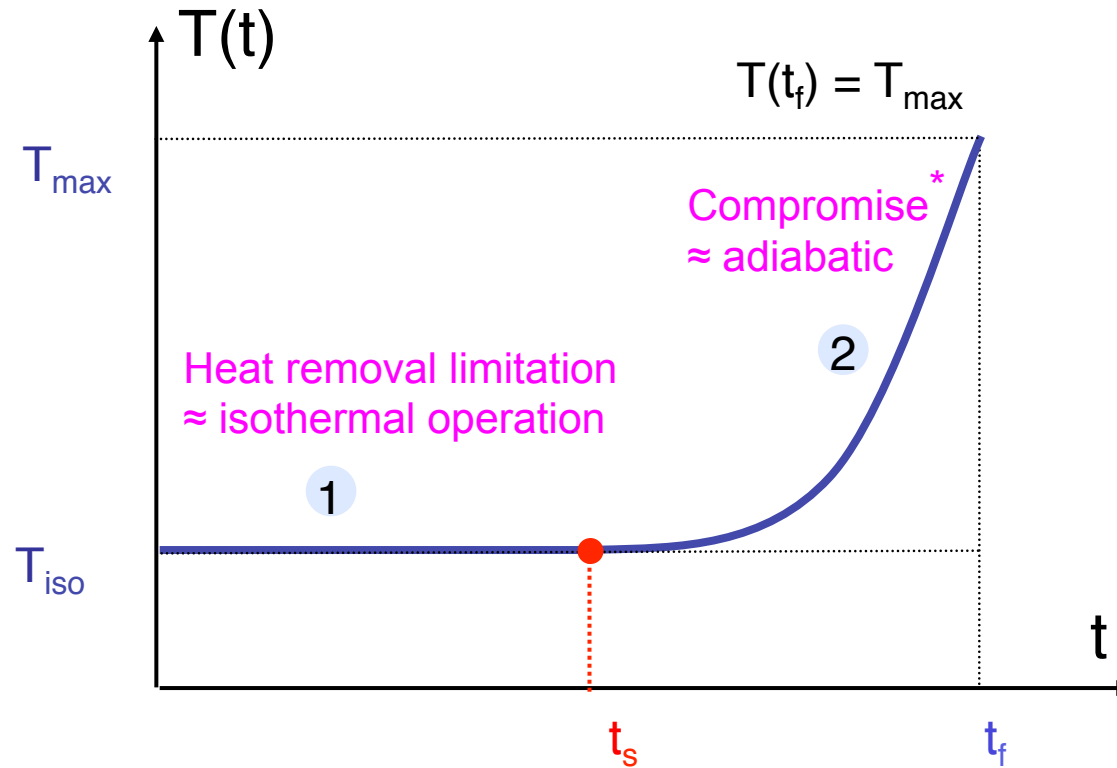
Numerical Solution using a Tendency Model



- 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
 \approx adiabatic*

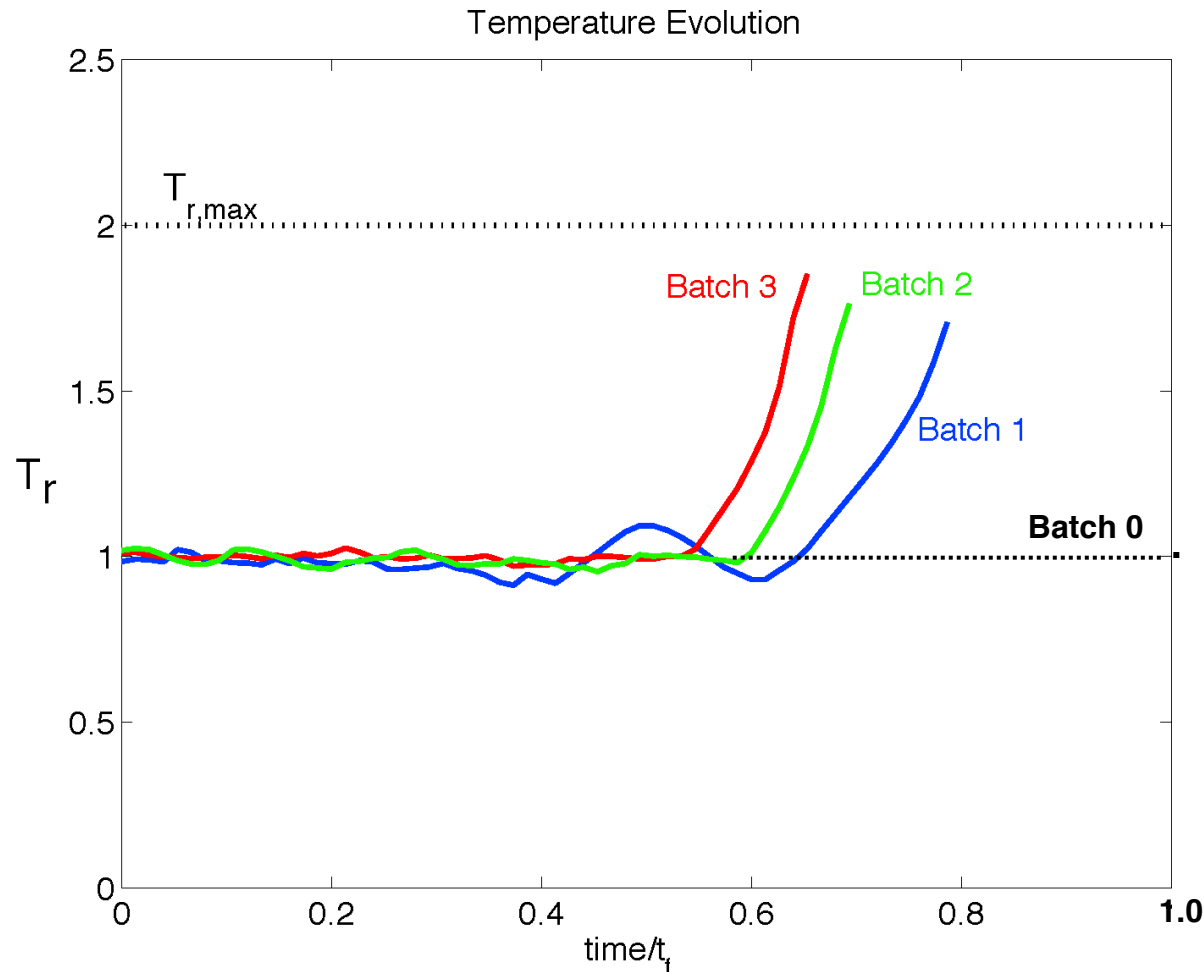
* Compromise between
conversion and quality

Heat removal limitation
 \approx isothermal operation

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

run-to-run adjustment of t_s

Industrial Results with NCO Tracking



AQUA+TECH

SPECIALTIES SA

1-ton reactor

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

Process optimization is difficult in practice

- Models are often inaccurate → use real-time measurements
- Repeated estimation and optimization lacks **model adequacy**
- Which measurements? How to best exploit them?
→ NCO (**active constraints and reduced gradients**)

Two approaches involving the NCO

- Input-affine corrections to cost and constraints
- NCO tracking (optimization via a multivariable control problem)
- Key challenge is **estimation of plant gradient**

NCO tracking

New Paradigm for RTO

Operator-friendly approach

- Start with best current operation (nominal model-based solution) and **push the process** until constraints are reached
- Know what to manipulate → **solution model**
- Determine how much to change from **measurements**

Important features

- Two steps: offline (model-based), online (data-driven)
- Can test **robustness** offline by using model perturbations
- Approach converges to **plant optimum**, not model optimum
- Complexity depends on the **number of inputs** (not system order)
- Solution is partly determined by active constraints → easy tracking
- Price to pay: need to **estimate experimental gradients**