Setting the Standard for Automation™

ISA France

Real-Time Optimization of Industrial Processes

Dominique Bonvin

Laboratoire d'Automatique

EPFL, Lausanne

En partenariat avec

IstiA

RUFEREQ

EPFL
ÉCOLE POLYTECHNIQUE
FÉDÉRALE DE LAUSANNE

Maîtrise et optimisation des processus complexes – Angers - 22 octobre 2014

Outline

1. **Optimization of process operation**

   – Numerical vs. real-time optimization

   – Static optimization for continuous and batch plants

2. **Real-time optimization schemes**

   – Two explicit strategies (repeat numerical optimization)

   – One implicit strategy (use feedback control)

3. **Experimental cases studies**

   – Fuel-cell stack (a continuous plant)

   – Batch polymerization (a batch plant)

4. **Conclusions**

Ideas

Concepts

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, Flow Rates, Compositions

→ Control

Measurements ↑

Manipulated Variables ↓

Large-scale complex processes

Changing conditions
→ Real-time adaptation
of set points

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

Plant
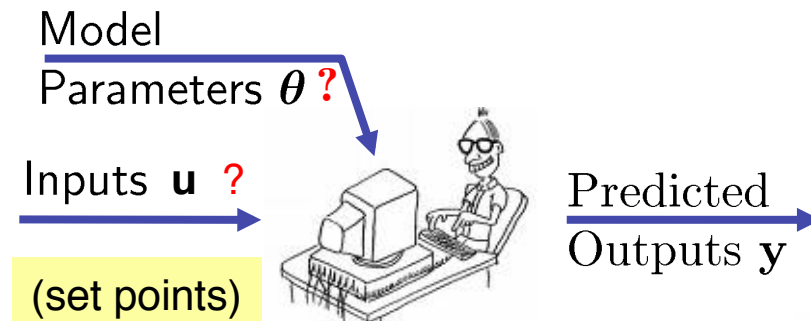
$$\min_{\mathbf{u}} \quad \phi_p(\mathbf{u}, \mathbf{y}_p)$$

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

Model-based Numerical Optimization

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

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

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

NLP

Inputs $\mathbf{u}$?

(set points)

Plant
Outputs $\mathbf{y_P}$

Model
Parameters $\boldsymbol{\theta}$?

Inputs $\mathbf{u}$?

(set points)

Predicted
Outputs $\mathbf{y}$

Optimization of a Batch Plant

Optimize the dynamic performance of a batch process
while satisfying a number of operational constraints

Batch unit with uncertainty regarding initial conditions, raw
material quality and model accuracy

$\mathbf{u}[0, t_f]$

$\mathbf{x}_p(t_f)$

Feed rate
Temperature

Productivity
Batch time

Uncertainty → Real-time adaptation of trajectories

Run-to-run Optimization of a Batch Plant
Problem formulation
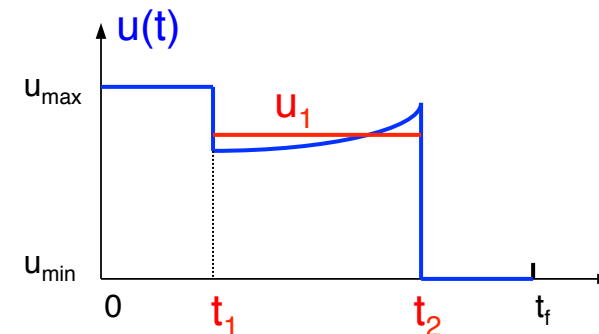

Batch plant with finite terminal time

$$\mathbf{u}(t) \longrightarrow \boxed{} \longrightarrow \mathbf{x}_p(t_f)$$

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

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

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

$$\mathbf{T}\big(\mathbf{x}(t_f)\big) \leq \mathbf{0}$$

Input Parameterization

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

$$\boldsymbol{\pi} \longrightarrow \boxed{} \longrightarrow \begin{array}{c} \Phi_p \\ \mathbf{G}_p \end{array}$$

Batch plant viewed as a static map

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

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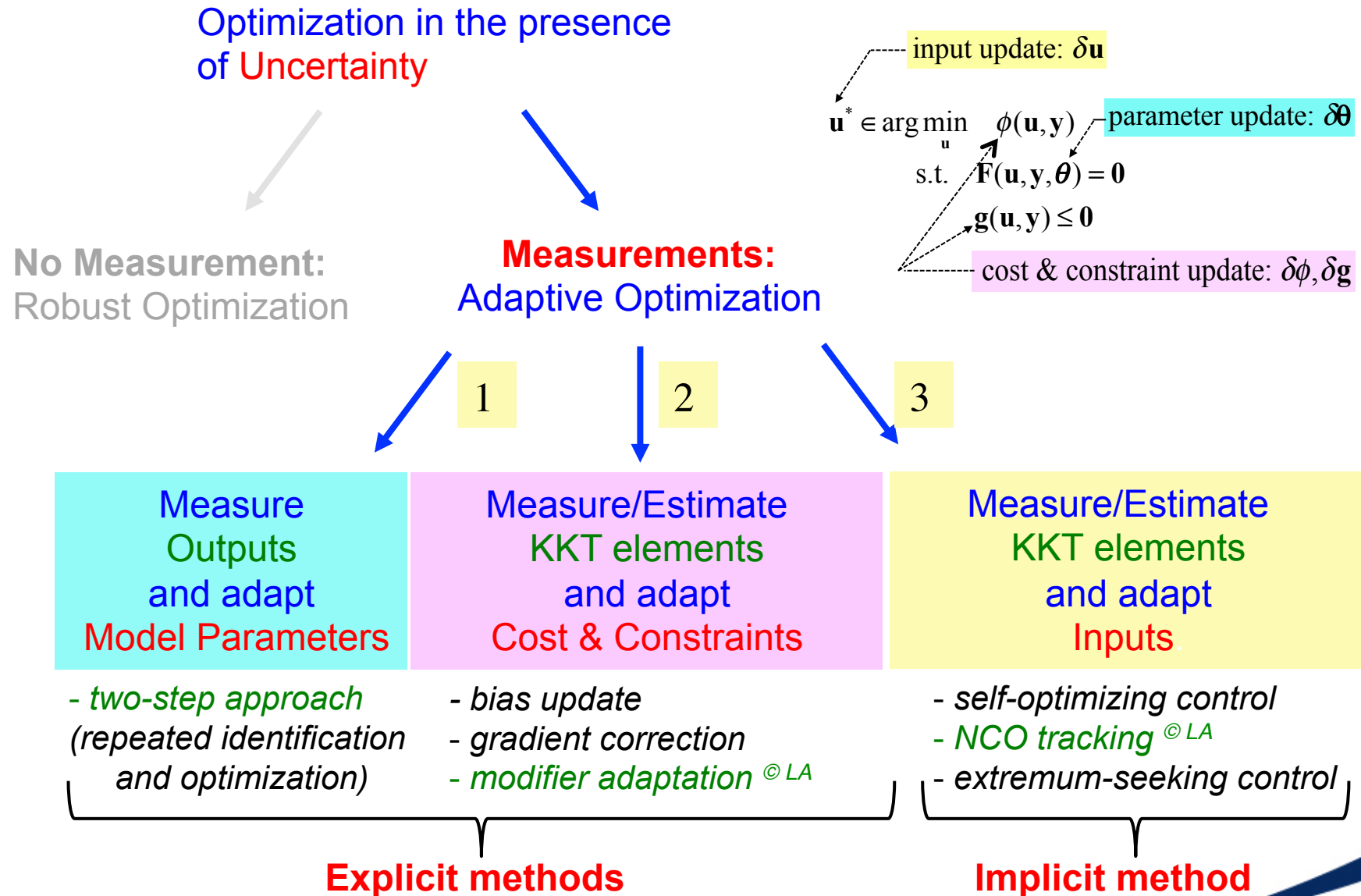
NLP

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Three Approaches for Static RTO
What to measure and what to adapt?

Optimization in the presence of Uncertainty

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

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

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

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

$$\mathbf{g}(\mathbf{u}, \mathbf{y}) \leq \mathbf{0}$$

cost & constraint update: $\delta \phi, \delta \mathbf{g}$

No Measurement: Robust Optimization

Measurements: Adaptive Optimization

| 1 | 2 | 3 |

| Measure Outputs and adapt Model Parameters | Measure/Estimate KKT elements and adapt Cost & Constraints | Measure/Estimate KKT elements and adapt Inputs |

- *two-step approach* (repeated identification and optimization)

- bias update
- gradient correction
- *modifier adaptation* © LA

- *self-optimizing control*
- *NCO tracking* © LA
- *extremum-seeking control*

Explicit methods

Implicit method

Two-step approach

Parameter Identification Problem

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

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

Optimization Problem

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

$$\mathrm{s.t.} \quad \mathbf{g}\left(\mathbf{u}, \mathbf{y}(\mathbf{u}, \boldsymbol{\theta}_k^*) \right) \leq \mathbf{0}$$

$$\mathbf{u}^{\mathrm{L}} \leq \mathbf{u} \leq \mathbf{u}^{\mathrm{U}}$$
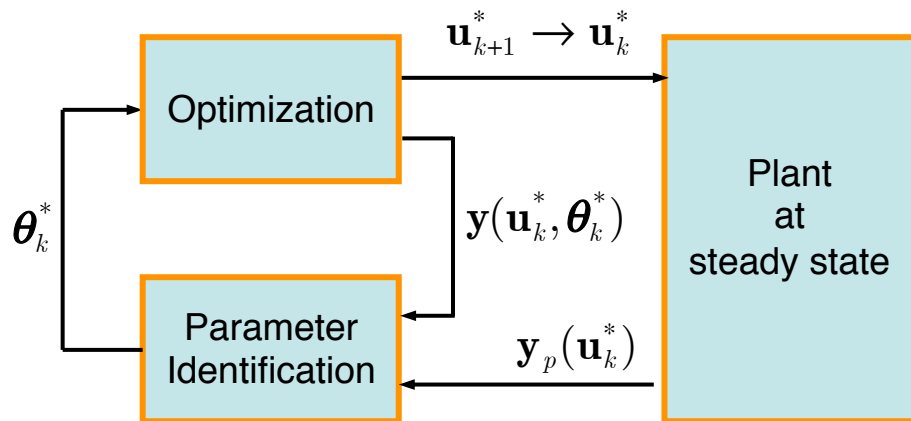
Current Industrial Practice
for tracking the changing optimum
in the presence of disturbances

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

Two-step Approach
With structurally incorrect model

$F_A, X_{A,\text{in}} = 1$ $F_B, X_{B,\text{in}} = 1$

T_R

V

$F = F_A + F_B$

$X_A, X_B, X_C, X_E, X_G, X_P$
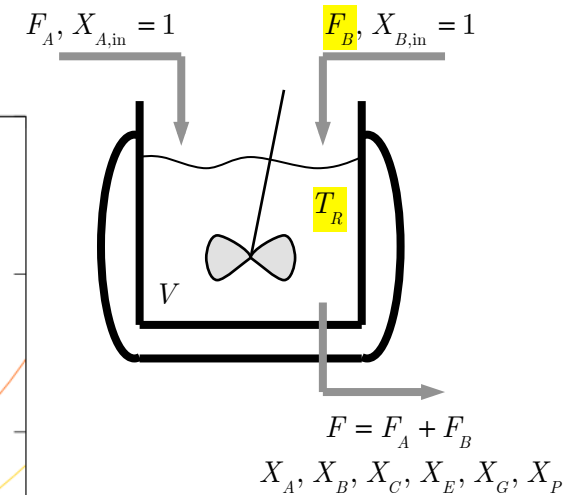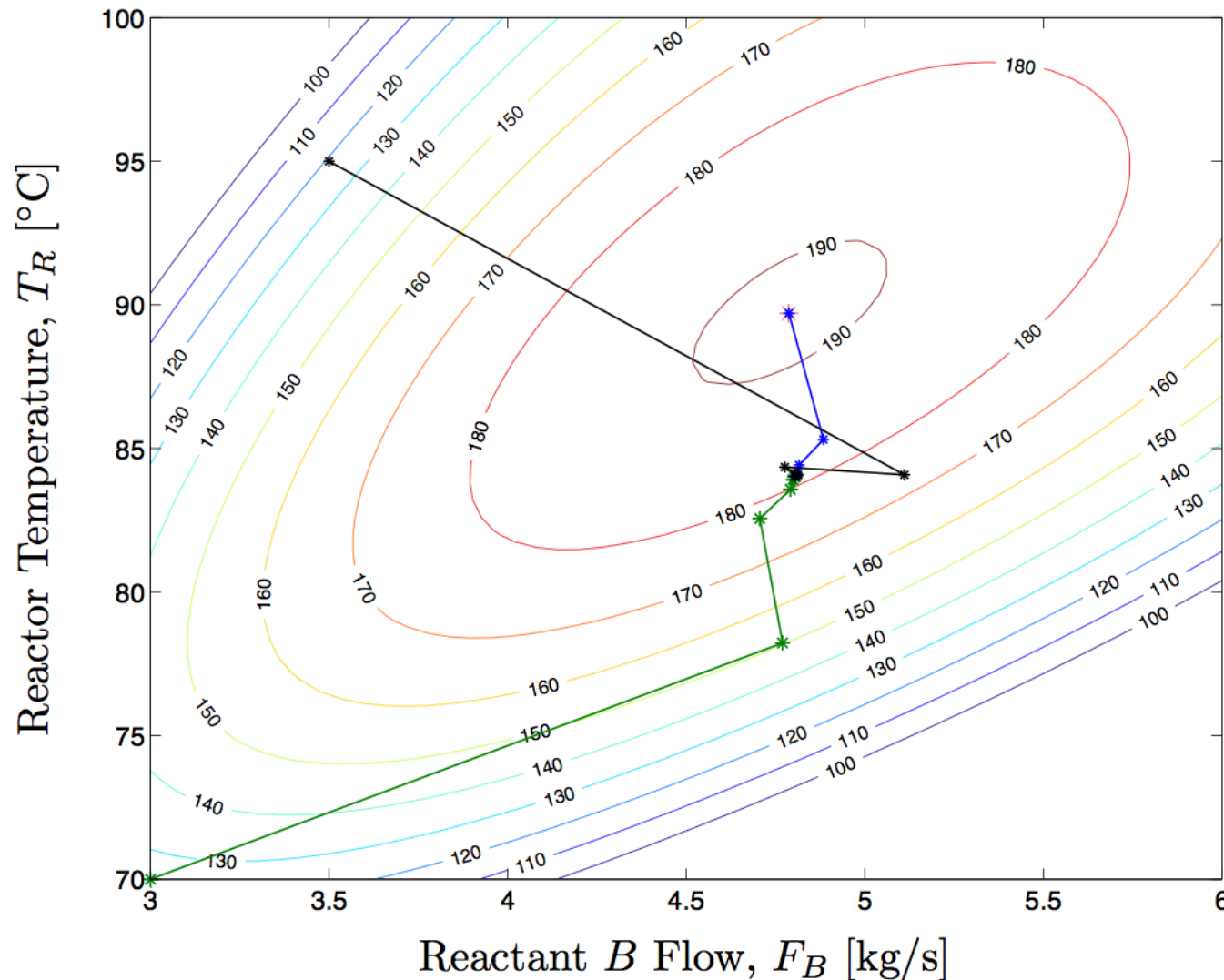
Williams-Otto Reactor
- 4$^{\text{th}}$-order model
- 2 inputs
- 2 adjustable par.

Does not converge to plant optimum

Modified Optimization Problem

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

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

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

Affine corrections of cost and constraint functions. The modified problem satisfies the first-order optimality conditions of the plant
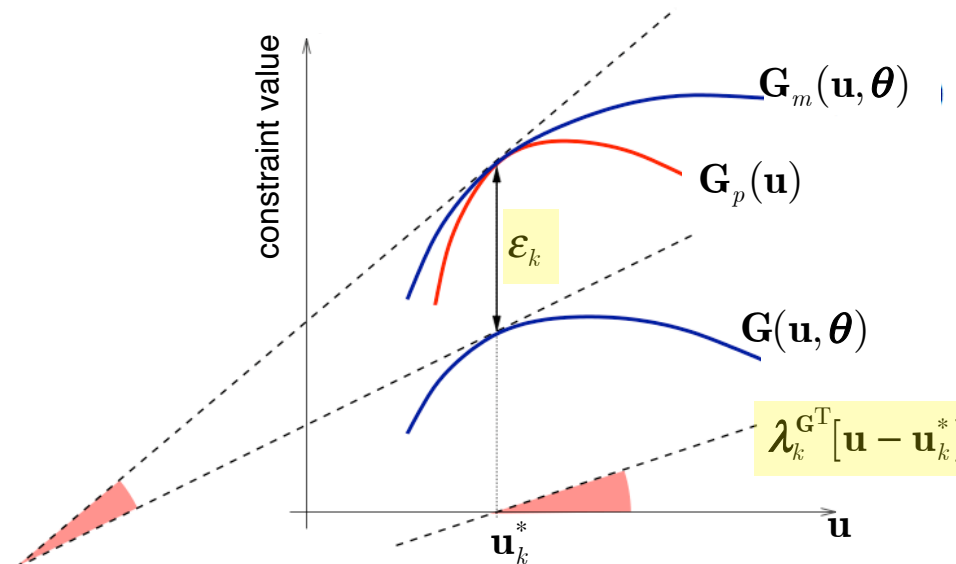
$$\boldsymbol{\lambda}_k^G = \frac{\partial \mathbf{G}_p}{\partial \mathbf{u}}(\mathbf{u}_k^*) - \frac{\partial \mathbf{G}}{\partial \mathbf{u}}(\mathbf{u}_k^*, \boldsymbol{\theta})$$

plant gradients

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

Modifier adaptation © LA

$F_A, X_{A,in} = 1$ $F_B, X_{B,in} = 1$

T_R

V

$F = F_A + F_B$

$X_A, X_B, X_C, X_E, X_G, X_P$
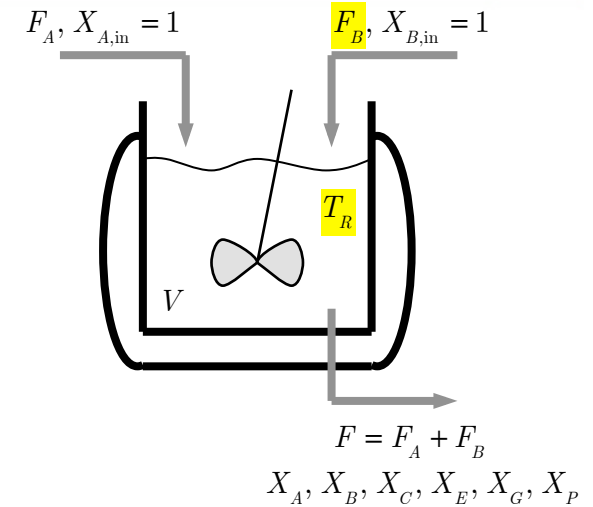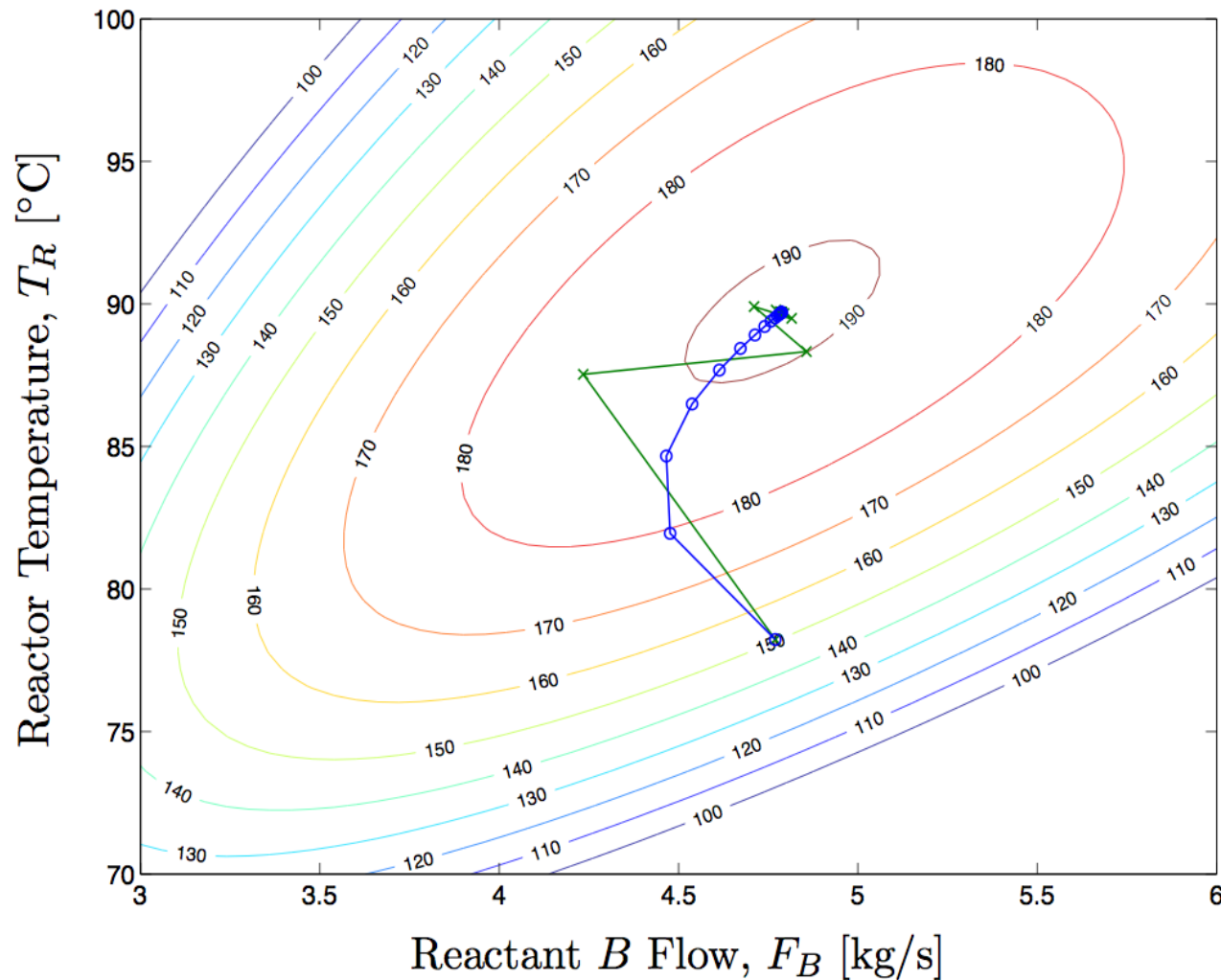
Williams-Otto Reactor
- 4th-order model
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- 2 adjustable par.

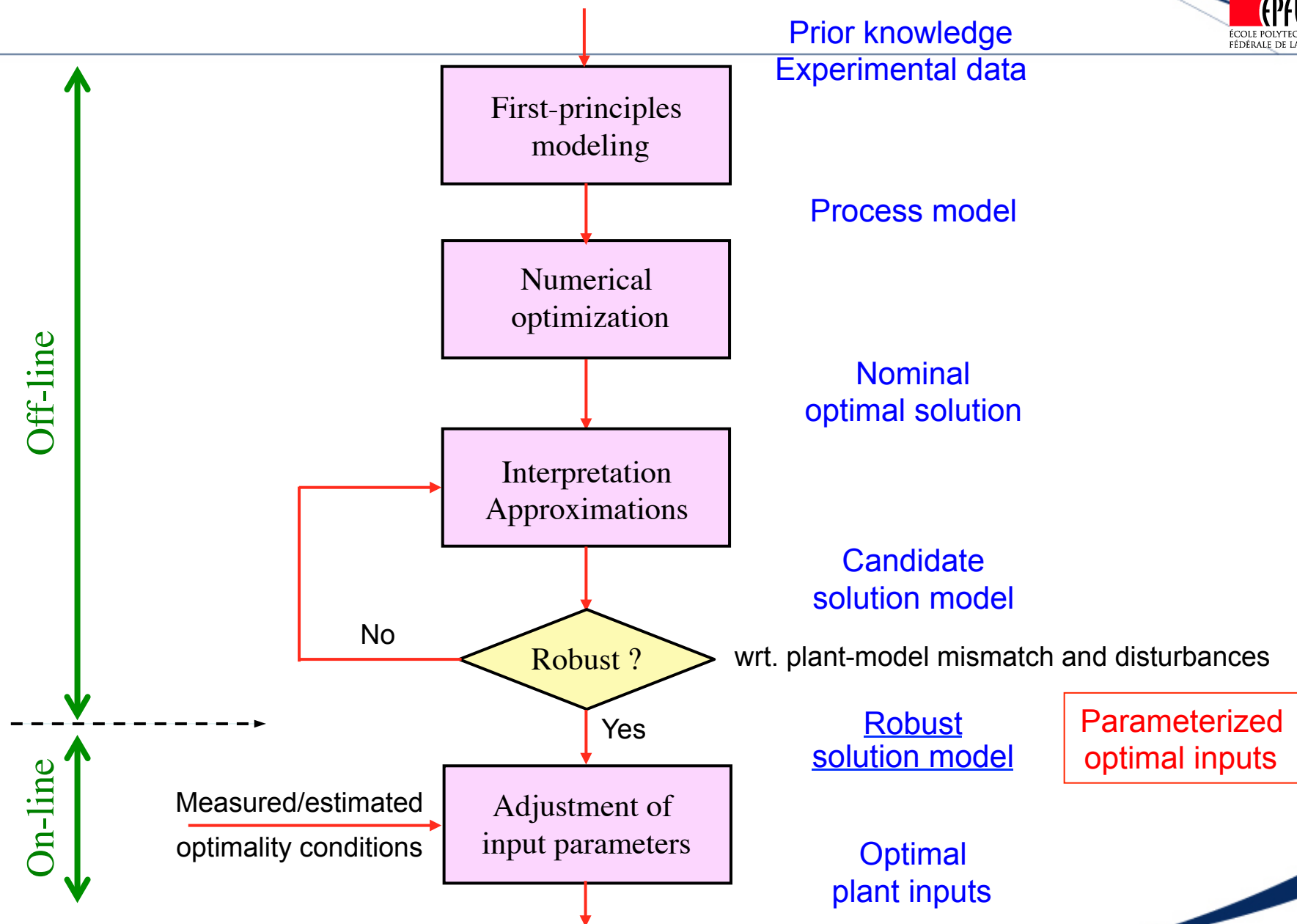Converges to plant optimum

Requires estimation of experimental gradient

A. Marchetti, PhD thesis, EPFL, *Modifier-Adaptation Methodology for Real-Time Optimization*, 2009

– Transform the optimization problem into a control problem

– Which setpoints to track for optimality?

   – The optimality conditions (active constraints, gradients)

   – Requires corresponding measurements

CV ?   **MV ?**

Set points ? → | Optimizing Controller | Inputs ? → | Real Plant | ← Disturbances

Measurements ?

Feasibility ?
Optimal performance ?

Solution model

Control problem
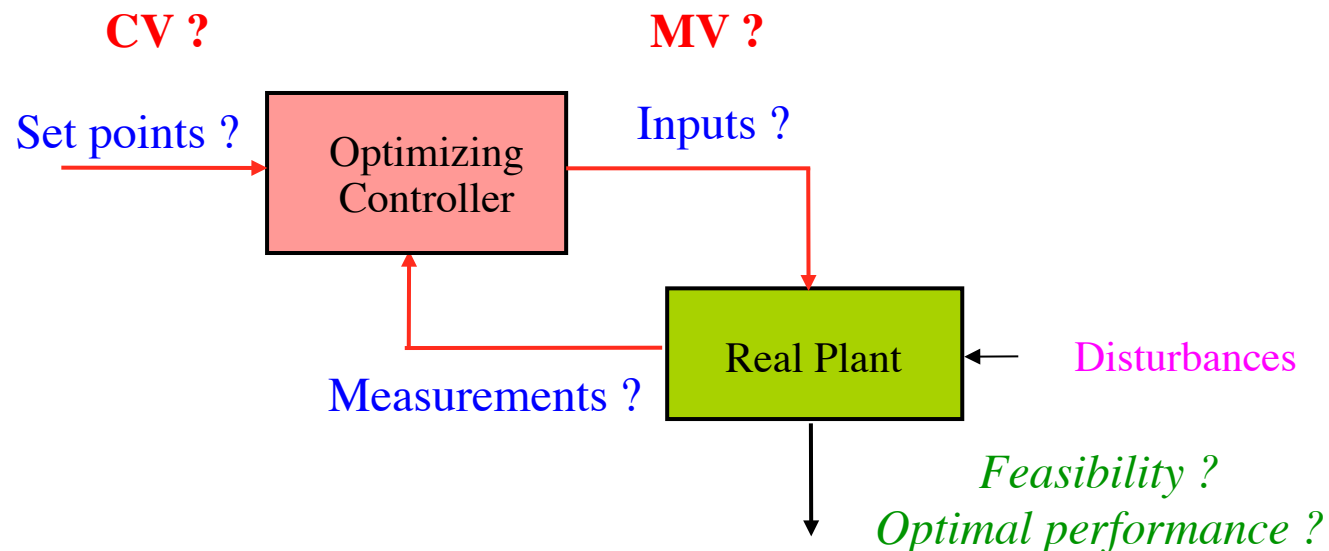
Generation of a Solution Model

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   – Batch polymerization (a batch plant) --   Approach 3

4. Conclusions

Ideas

Concepts

Solid Oxide Fuel Cell Stack

RTO via modifier adaptation © LA

$$H_2 + \frac{1}{2} O_2 \rightarrow H_2O$$
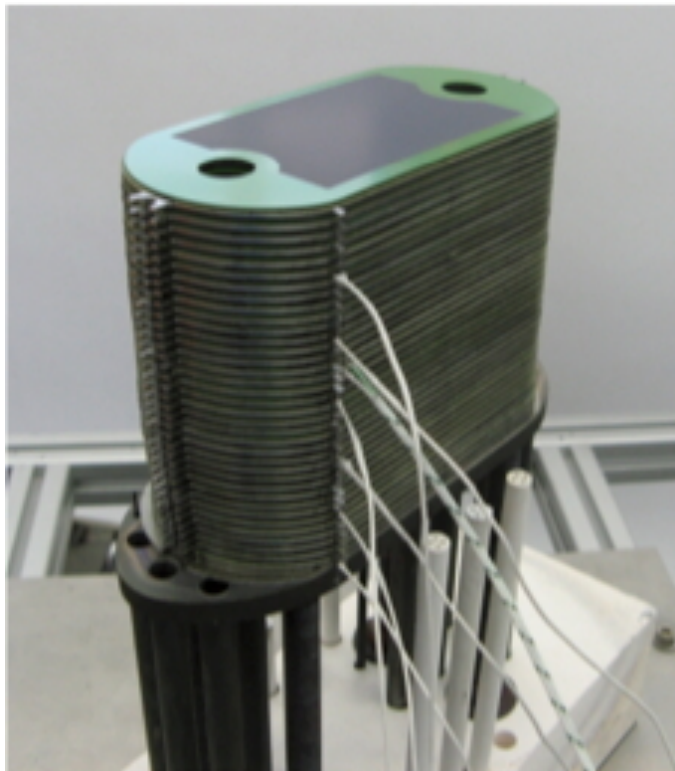
- Stack of 6 cells, active area of 50 cm², metallic interconnector
- Anodes : standard nickel/yttrium stabilized-zirconia (Ni-YSZ)
- Electrolyte : dense YSZ.
- Cathodes: screen-printed (La, Sr)(Co, Fe)O₃
- Operation temperatures between 650 and 850°C.
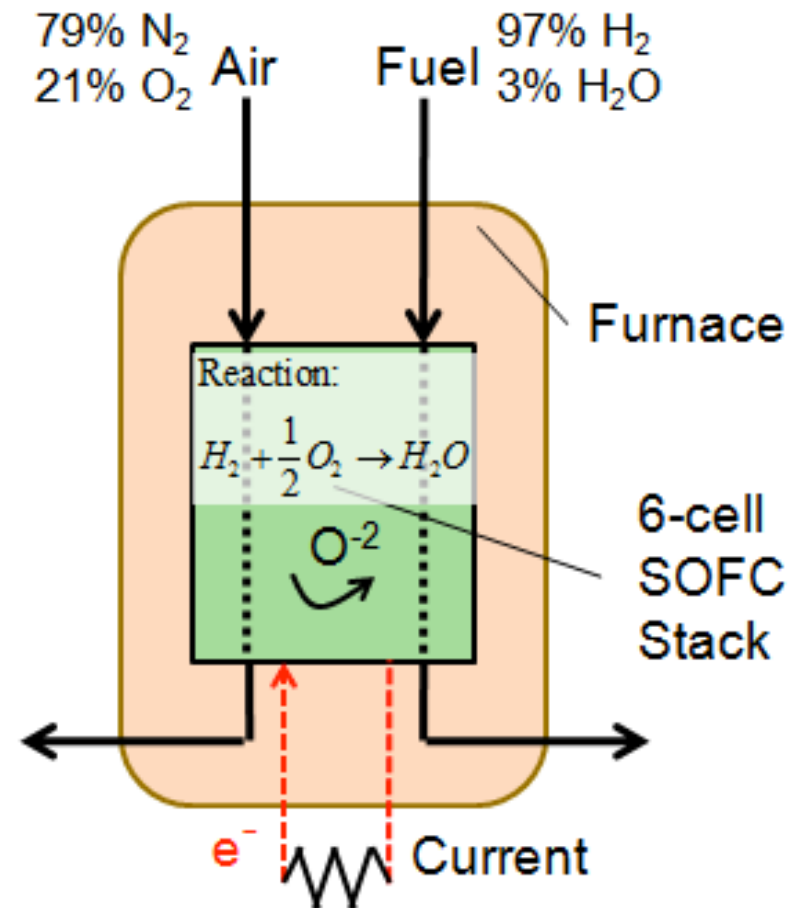
Experimental Features

- **Objective:** maximize electrical efficiency

- Meet power demand that changes unexpectedly

- **Inputs:** flowrates of H_2 and O_2, current

- **Outputs:** power density, cell potential

- Time-scale separation

  - *slow temperature dynamics, treated as process drift !*

  - *static model (for the rest)*

- Inaccurate model in the operating region (power, cell)

G.A. Bunin *et al.*, Experimental Real-Time Optimization of a Solid Oxide Fuel Cell Stack via Constraint Adaptation, *Energy,* 39(1), 54-62, 2012

Repeated Numerical Optimization

- Solve a static optimization problem every 10 sec
- Apply the optimal inputs to the fuel cell stack
- Measure the resulting constraint values
- Adapt the modifiers ε to match the active constraints

$$\max_{u_k} \quad \eta\left(\mathbf{u}_k, \boldsymbol{\theta}\right)$$

$$\text{s.t.} \quad \boldsymbol{p}_{el}\left(\mathbf{u}_k, \boldsymbol{\theta}\right) + \varepsilon_{k-1}^{p_{el}} = \boldsymbol{p}_{el}^{s}$$

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

$$\nu\left(\mathbf{u}_k\right) \leq 0.75$$

$$4 \leq \lambda_{air}\left(\mathbf{u}_k\right) \leq 7$$

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

$$\boldsymbol{u}_{3,k} \leq 30\text{A}$$

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

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

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

Experimental Results

- Random power changes every 5 min

- RTO every 10 sec, matches the active constraints at steady state
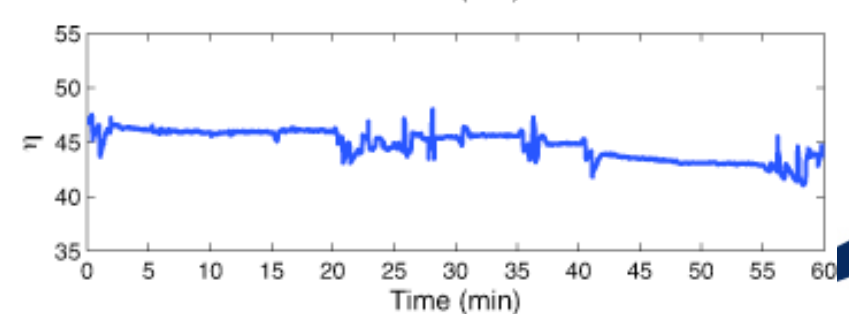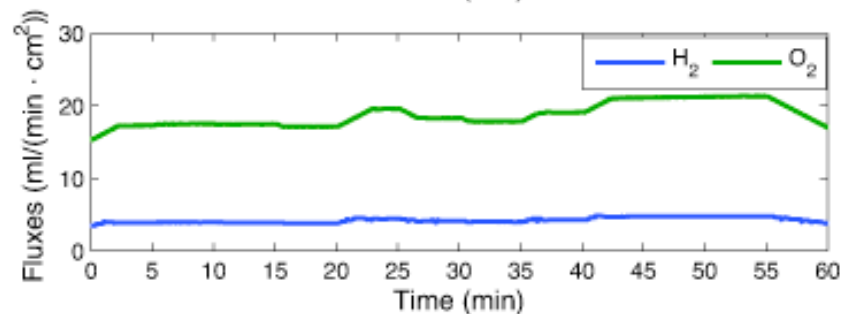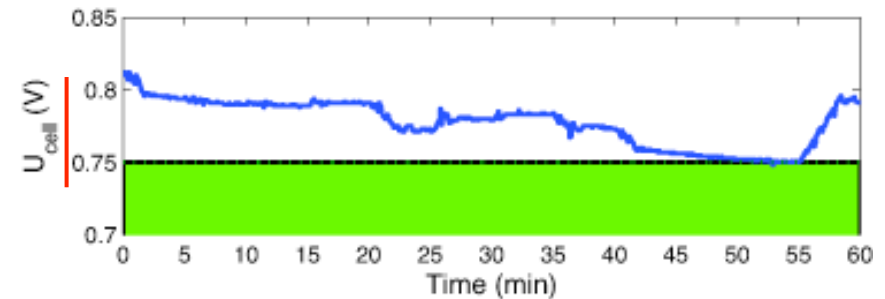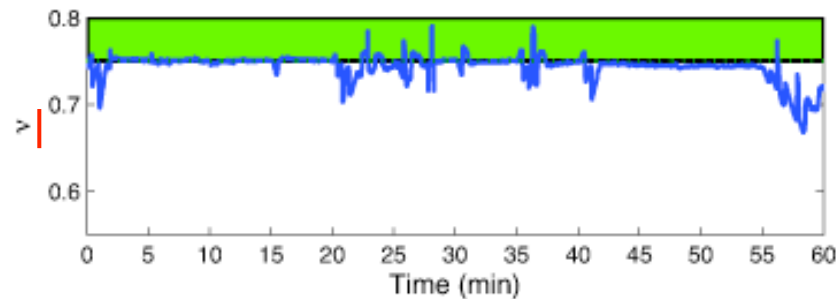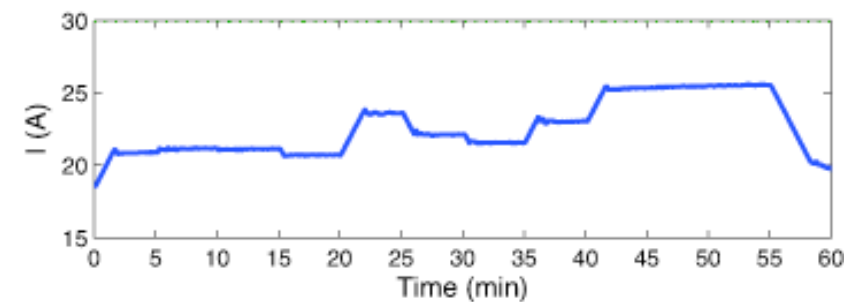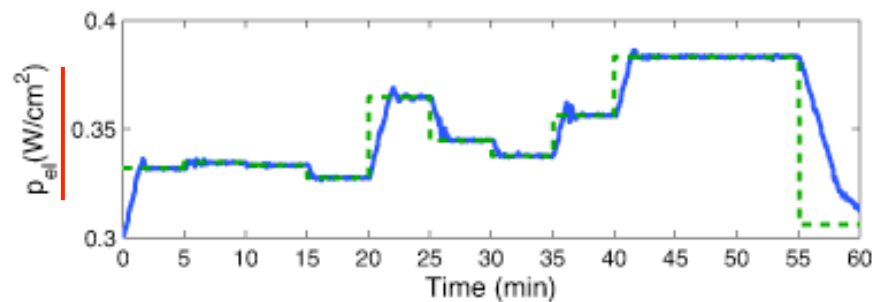
Optimization of Polymerization Reactor
NCO tracking © LA

- Industrial features

  - 1-ton reactor, risk of runaway

  - Initiator efficiency can vary considerably

  - Several recipes

    ➢ *different initial conditions*

    ➢*different initiator feeding policies*

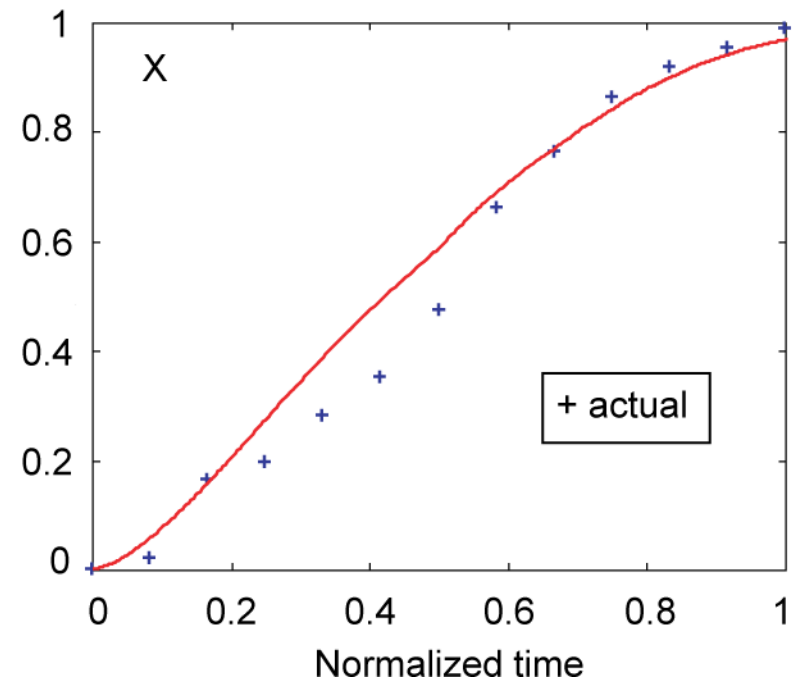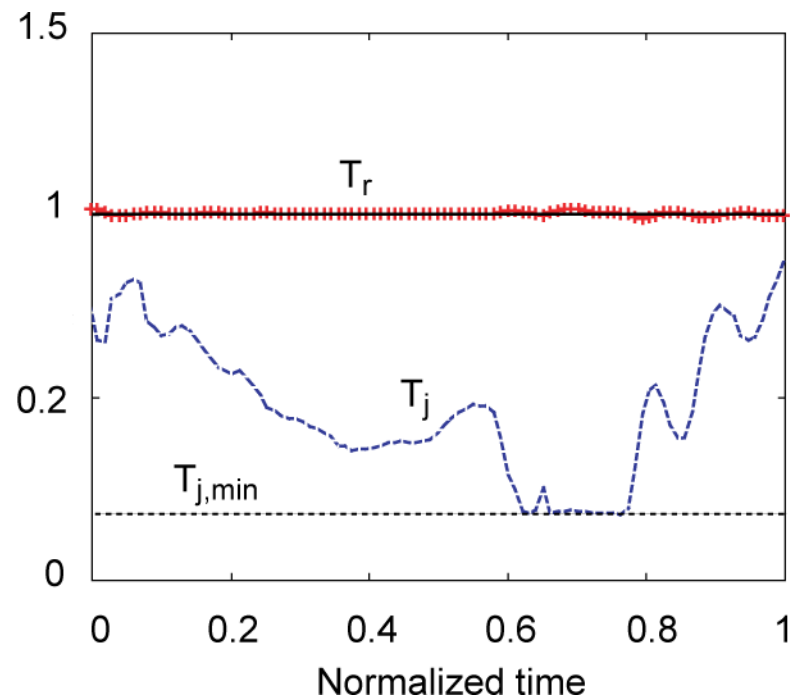   ➢ *use of chain transfer agent*

    ➢*use of reticulant*

➡ • Modeling difficulties
  • Uncertainty

- Challenge: Implement (near) optimal operation for various recipes

G. François *et al.*, Run-to-Run Adaptation of a Semi-Adiabatic Policy for the Optimization of an Industrial Batch Polymerization Process, *I&ECResearch*, *43*, 7238-7242 (2004)
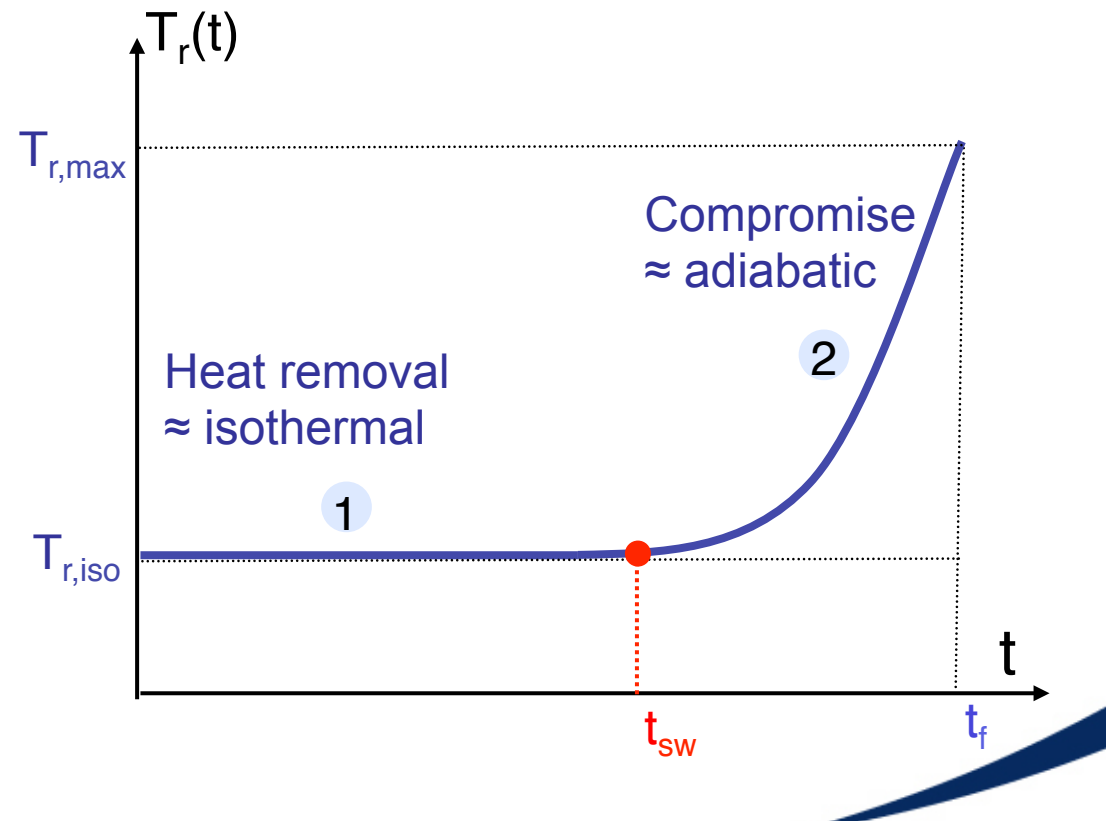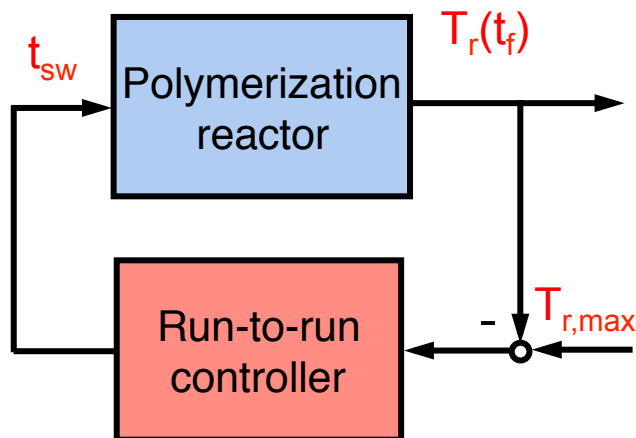
Industrial Practice

$T_r(t)$ to minimize the batch time ?
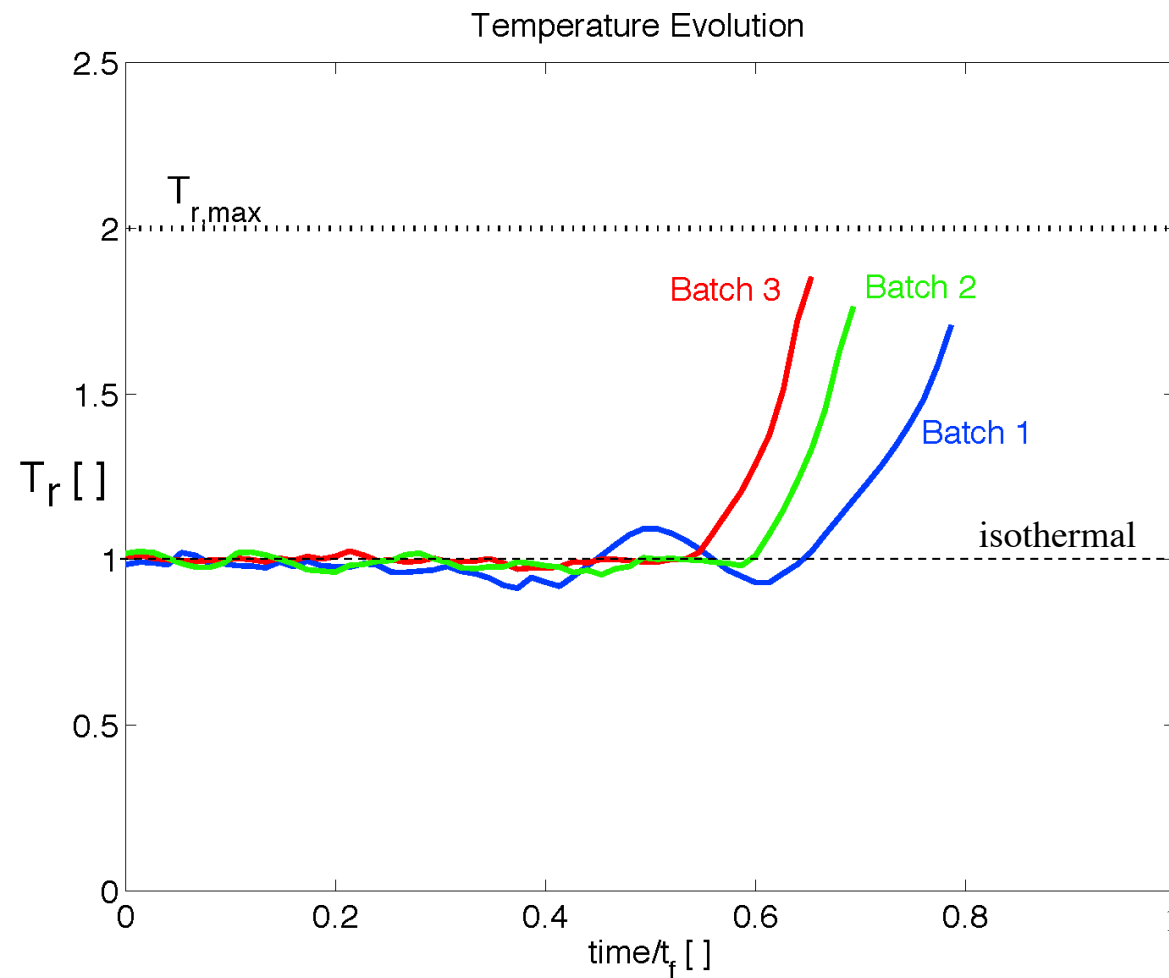
Strategy for Run-to-run Optimization

Tendency model

Optimality is linked with meeting the most restrictive constraint $T_r(t_f) = T_{r,max}$

Strategy: Manipulate t_{sw} on a run-to-run basis to force $T_r(t_f)$ at $T_{r,max}$

Industrial Results

Temperature Evolution

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

Conclusions

- Process models are often <u>inadequate for optimization</u>

    → use real-time measurements for appropriate adaptation

- Which measurements to use? How to best exploit them?

    o Outputs: easily available, not necessarily appropriate

    o KKT modifiers allow meeting KKT conditions

    ➢ modifier adaptation (explicit optimization)

    ➢ NCO tracking (implicit optimization

- Key challenge is estimation of plant gradient