Real-Time Optimization in the Presence of Uncertainty

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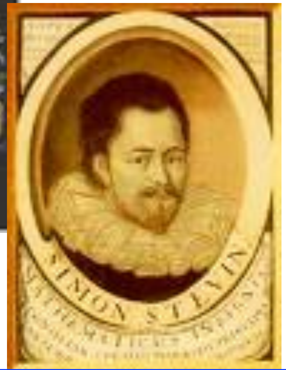
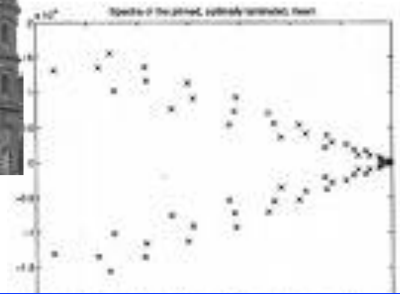
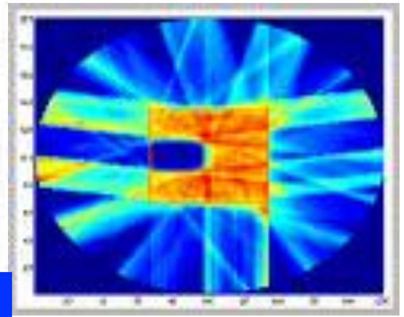
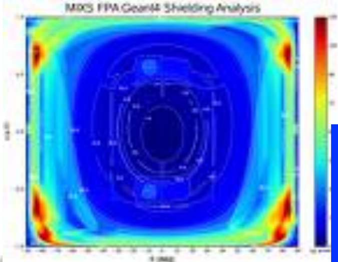
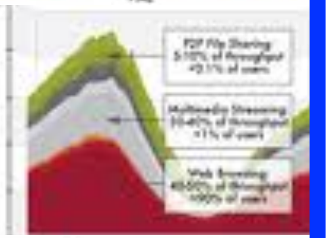




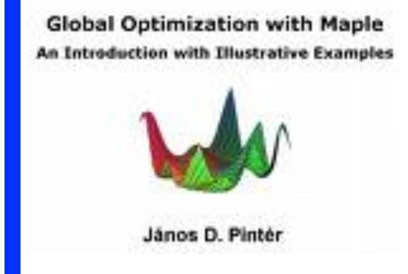


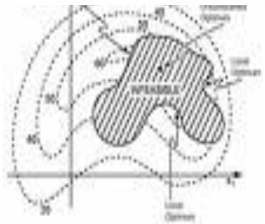


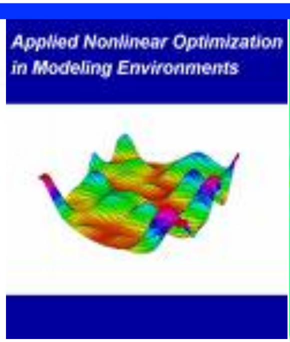


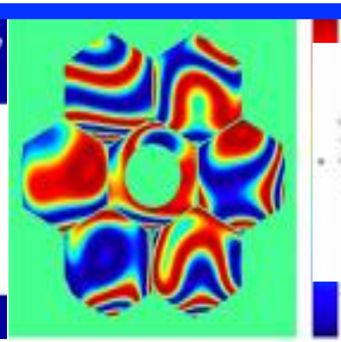
Optimization of process operation

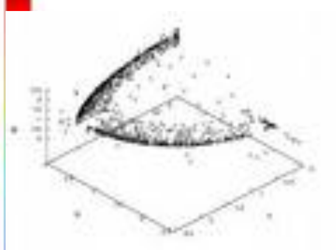
- **Static optimization u** *RTO*
  - steady-state performance of dynamic processes
  - run-to-run operation of batch processes
- **Dynamic optimization u*(t)*** *DRTO*
  - transient behavior of dynamic processes

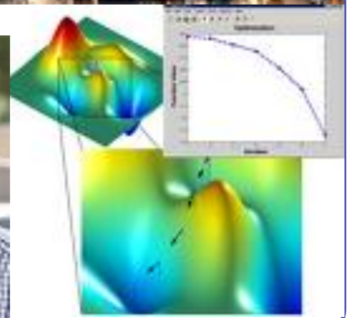












Outline

Context of uncertainty

- Plant-model mismatch
- Disturbances

→ Use measurements for process improvement

Static optimization

- *Adaptation of model parameters* – Repeated identification & optimization
- *Adaptation of cost and constraints* – Modifier adaptation
- *Direct adaptation of inputs* – NCO tracking

Application examples

Real-Time Optimization of a Continuous Plant

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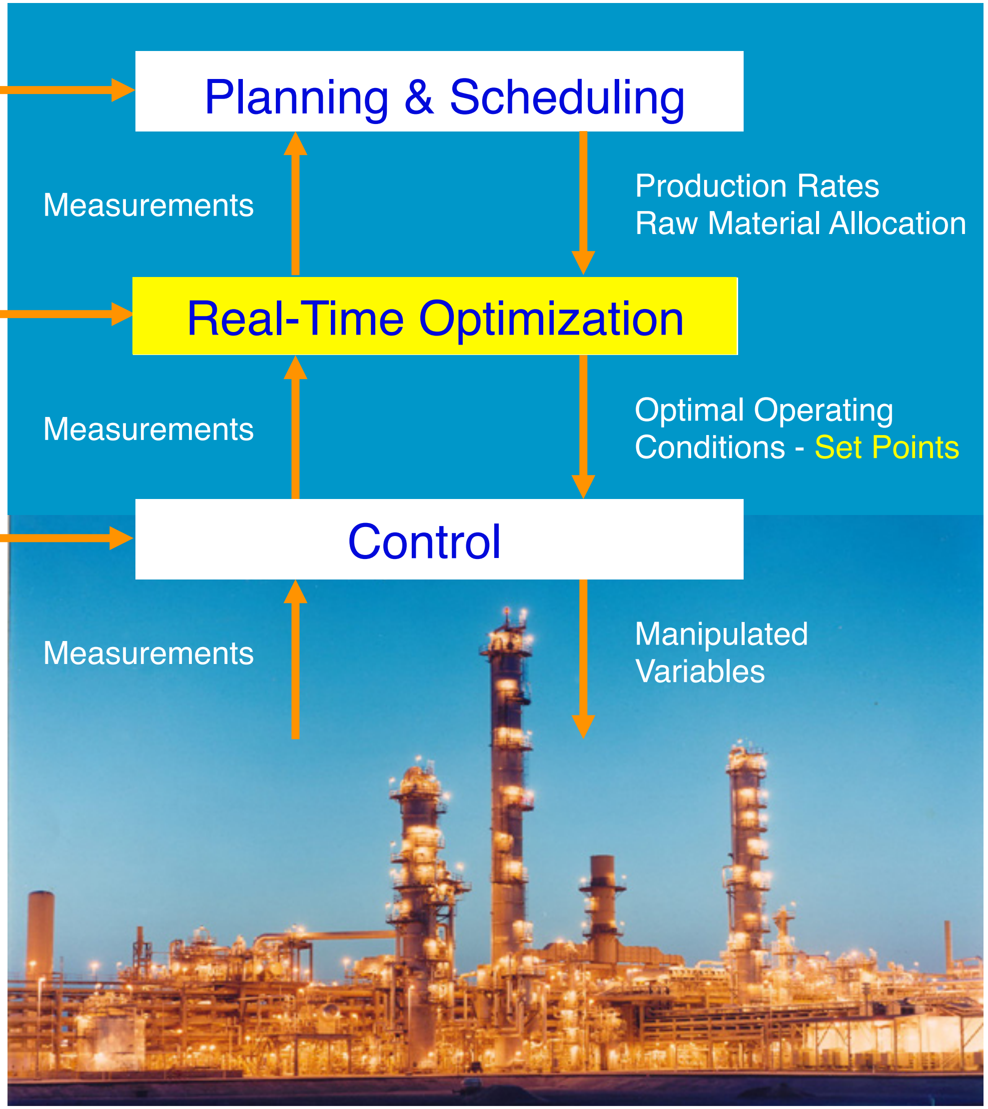
	Disturbances
Long term week/month	Market Fluctuations, Demand, Price
Medium term day	Catalyst Decay, Changing Raw Material Quality
Short term second/minute	Fluctuations in Pressure, Flowrates, Compositions

Decision Levels

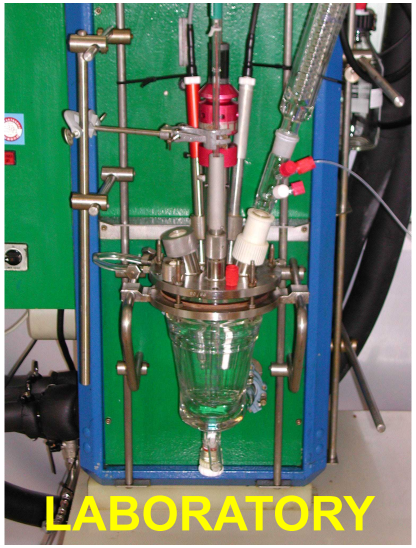


Large-scale complex processes

Changing conditions
➔ Real-time adaptation

Optimization of a Discontinous Plant

RECIPE → BATCH PLANT → PRODUCTS



Differences in Equipment and Scale

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

Scale-up

Production Constraints

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

Different conditions ➔ Run-to-run adaptation

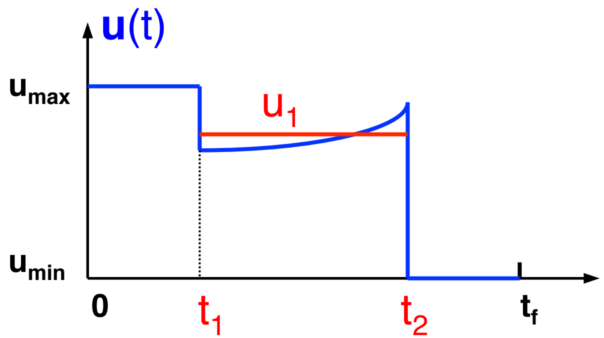
Run-to-Run Optimization of a Batch Plant

Batch plant with
finite terminal time

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

Input Parameterization

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



Batch plant
viewed as a static map

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

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

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

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

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*

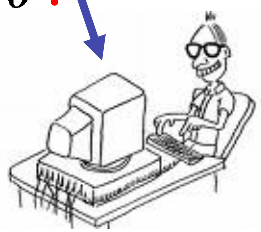
* corresponding KKT conditions (first-order NCO)

Inputs $\mathbf{u}$? (set points)

Plant Outputs $\mathbf{y}_p$

Model Parameters $\boldsymbol{\theta}$?

Inputs $\mathbf{u}$? (set points)



Predicted Outputs $\mathbf{y}$

Implementation Issues

Model, measurements and input parameters

- The nominal model is often too inaccurate to lead to plant optimality; hence the need to use measurements and implement adaptive optimization
- The model can be seen as a vehicle to process the available measurements and compute the optimal inputs
- What measurements to use (plant outputs vs. KKT elements)?
- What inputs to use (in particular when the input vector results from input parameterization)?
- Models are typically not trained to predict the KKT conditions

  → justifies the use of correction terms in adaptive optimization schemes

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Three Adaptation Options

Optimization in the presence of Uncertainty

No Measurement: Robust Optimization

Measurements: Adaptive Optimization

input adapt. $\delta \mathbf{u}$

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

parameter adapt. $\delta \boldsymbol{\theta}$

cost & const. adapt. $\delta \phi$, $\delta \mathbf{g}$

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

Adaptation of Model Parameters

- two-step approach of repeated identification and optimization

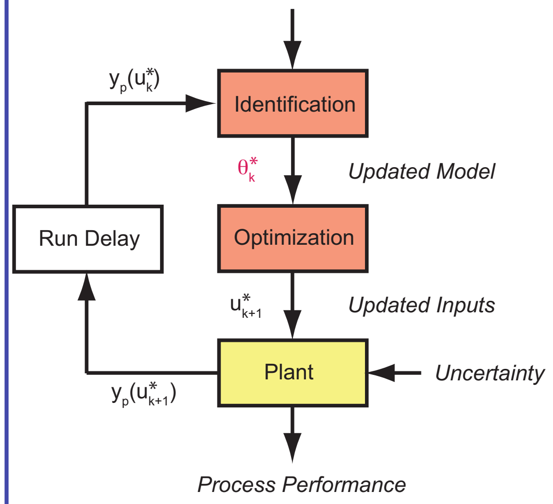
Adaptation of Cost & Constraints

- constraint correction
- gradient correction
- ISOPE

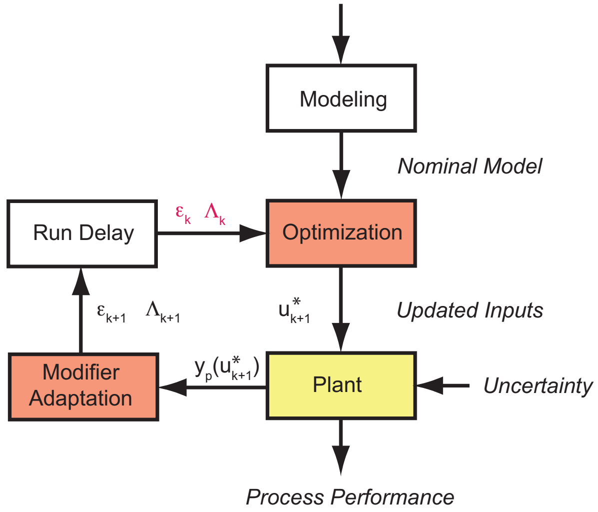
Adaptation of Inputs

- tracking active constraints
- gradient control
- NCO tracking
- self-optimizing control

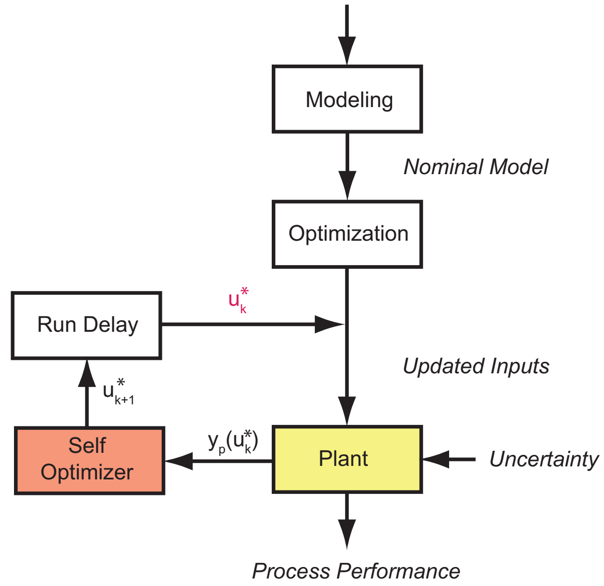
Three Iterative RTO Scenarios



Two-step approach



Cost & constraint adaptation
(Modifier adaptation)



NCO tracking

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1. Adaptation of Model Parameters

Repeated Identification and Optimization

Parameter Estimation Problem

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

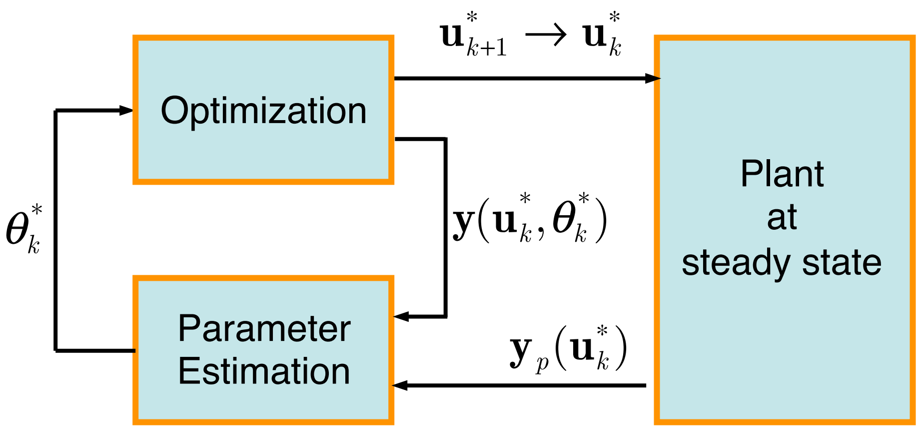
$$J_k^{\text{id}} = \left[\mathbf{y}_p(\mathbf{u}_k^*) - \mathbf{y}(\mathbf{u}_k^*, \theta)\right]^{\text{T}} \text{Q} \left[\mathbf{y}_p(\mathbf{u}_k^*) - \mathbf{y}(\mathbf{u}_k^*, \theta)\right]$$

Optimization Problem

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

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

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

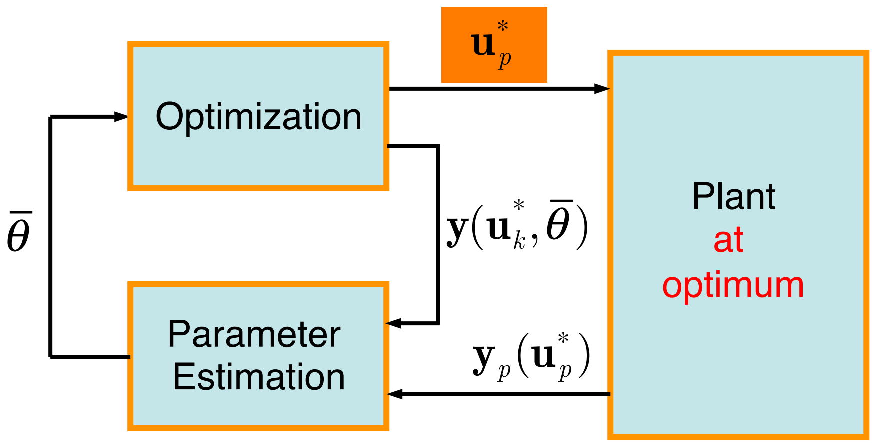


Current Industrial Practice
for tracking the changing optimum
in the presence of disturbances

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

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

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

SOSC

Par. Est.

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

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

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

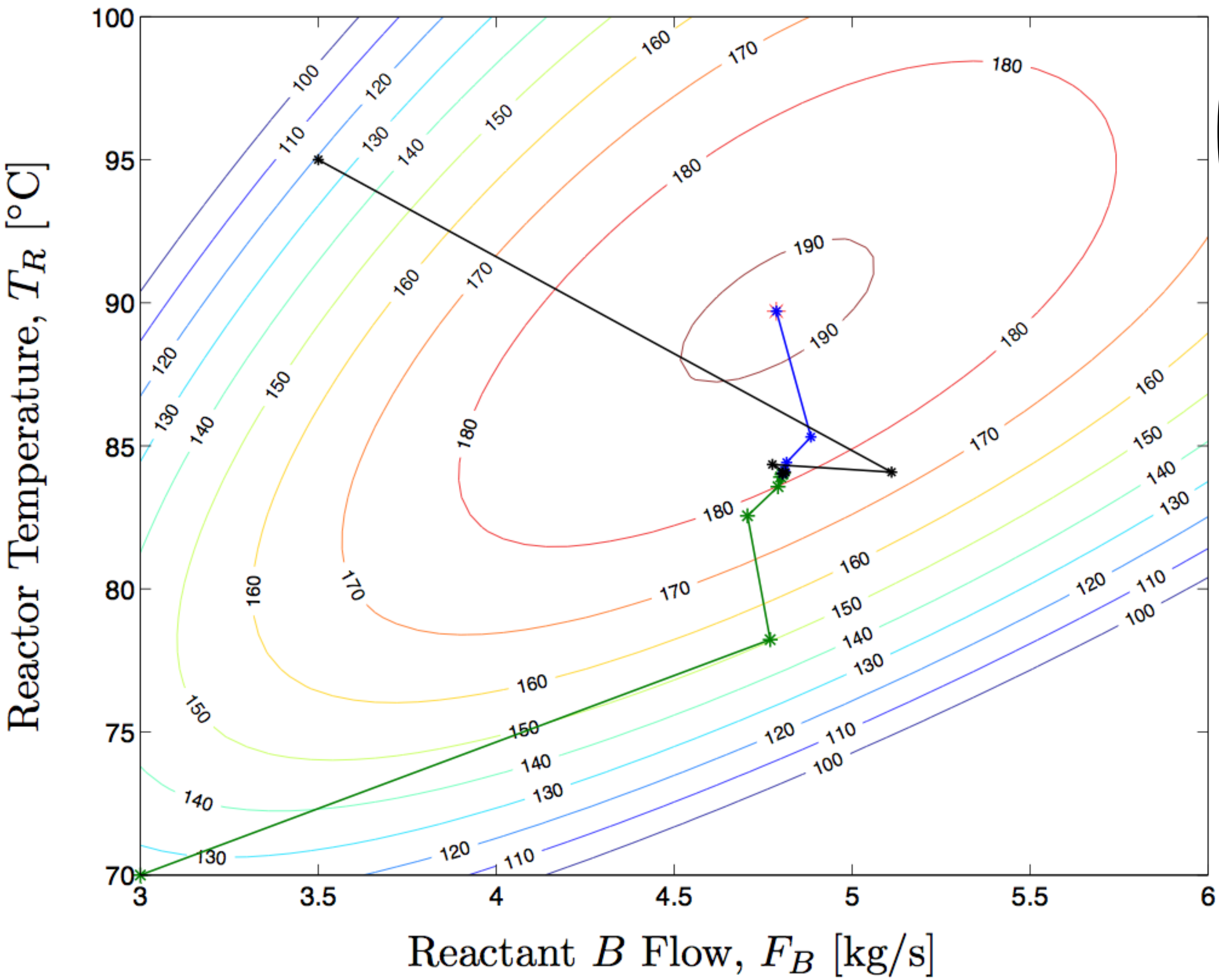
$$\nabla_r^2 \Phi(\mathbf{u}_p^*, \bar{\theta}) > 0$$

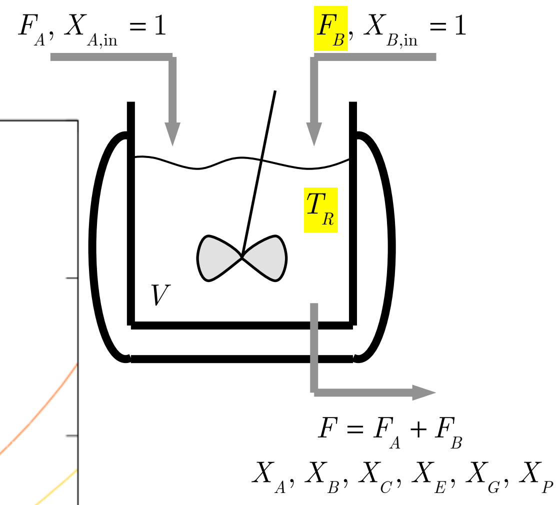
Opt.

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

Example of Inadequate Model

Two-step approach





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

Does not converge to plant optimum

T. J. Williams and R. E. Otto, A generalized chemical processing model for the investigation of computer control, *AIEE*, **79**, 458, 1960

2. Modifier Adaptation

Repeated Optimization using Nominal Model

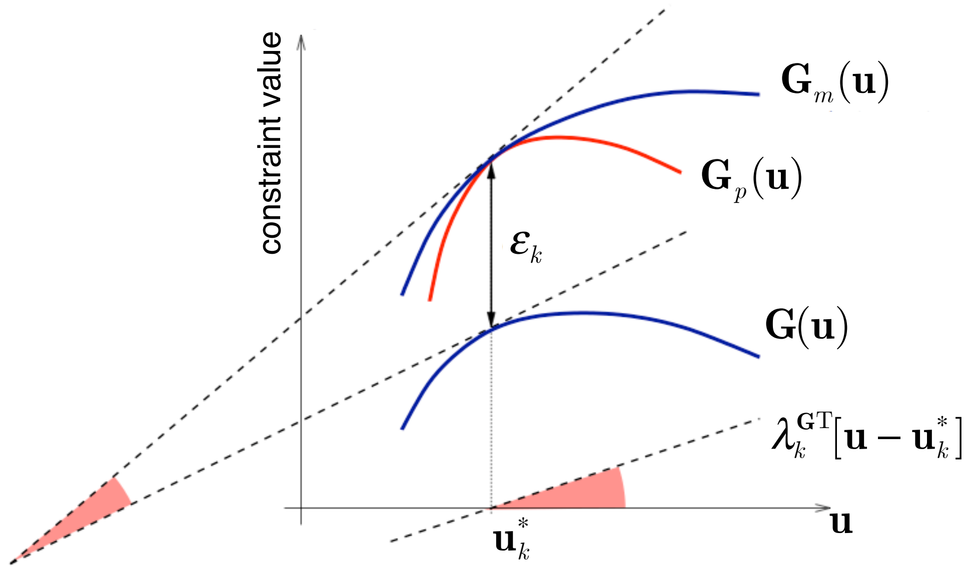
Modified Optimization Problem

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

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

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

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. Modifier Adaptation

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

Model Adequacy for Modifier Adaptation

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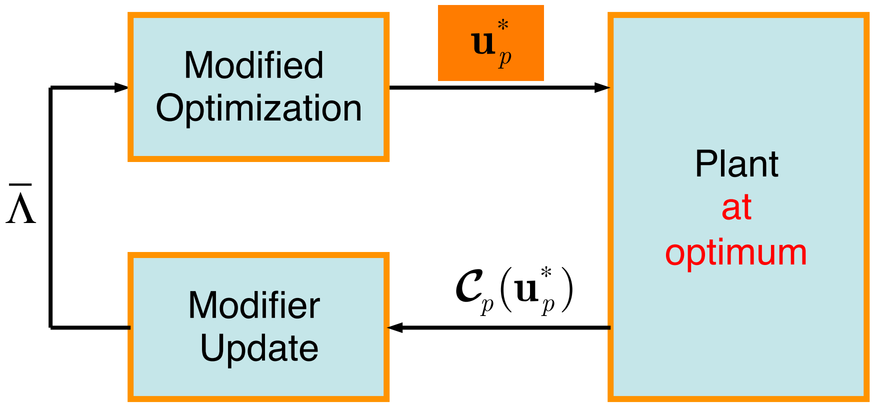

$$\bar{\Lambda} = \mathcal{C}_p(\mathbf{u}_p^*) - \mathcal{C}(\mathbf{u}_p^*)$$

Converged value

Model-adequacy condition

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

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

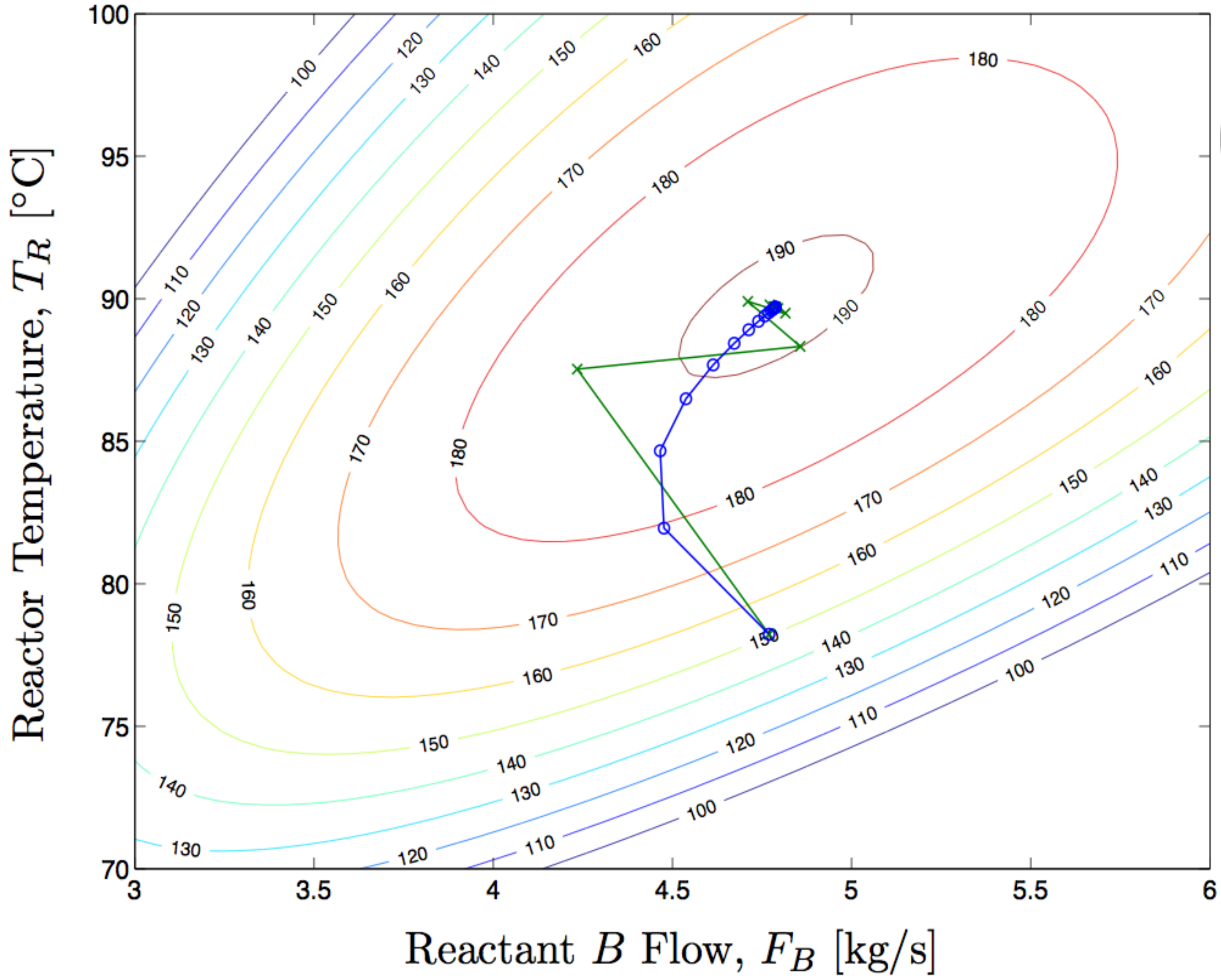
$$G_i(\mathbf{u}_p^*) < 0, \quad i \notin A(\mathbf{u}_p^*)$$

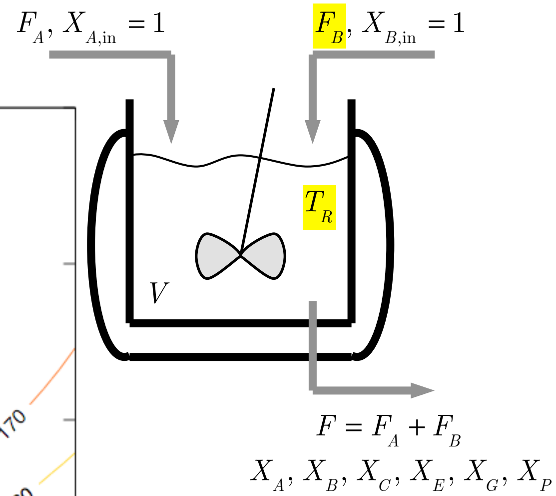
$$\nabla_r \Phi(\mathbf{u}_p^*) = \mathbf{0},$$

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

Example Revisited

Modifier adaptation





Williams-Otto Reactor

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

Converges to plant optimum

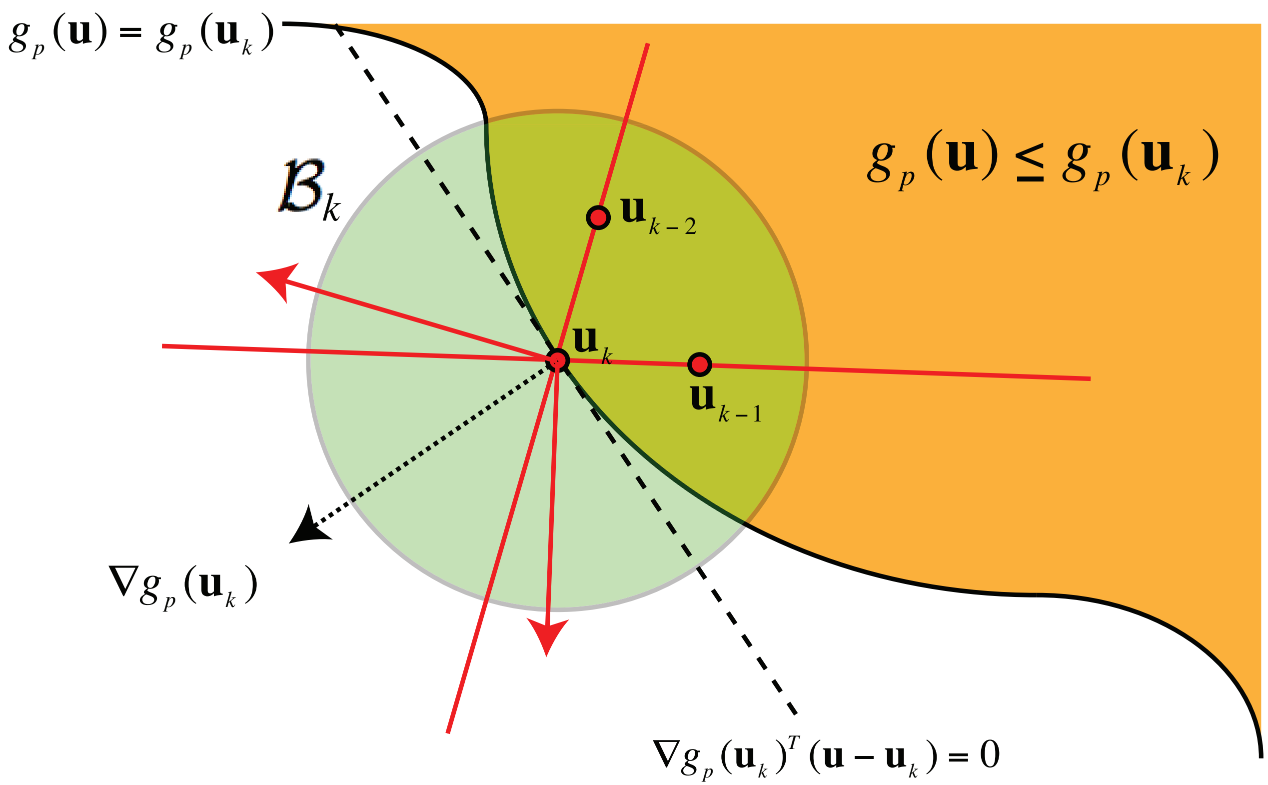
Alejandro Marchetti, PhD thesis, EPFL, *Modifier-Adaptation Methodology for Real-Time Optimization*, 2009

Requires Plant Gradients

Recent results

Regularize with convex/quasiconvex structures, which allows bounding the gradient and reducing the effect of noise.

G.A. Bunin, G. François and D. Bonvin, Exploiting local quasiconvexity for gradient estimation in modifier-adaptation schemes, *American Control Conference*, Montreal 2012



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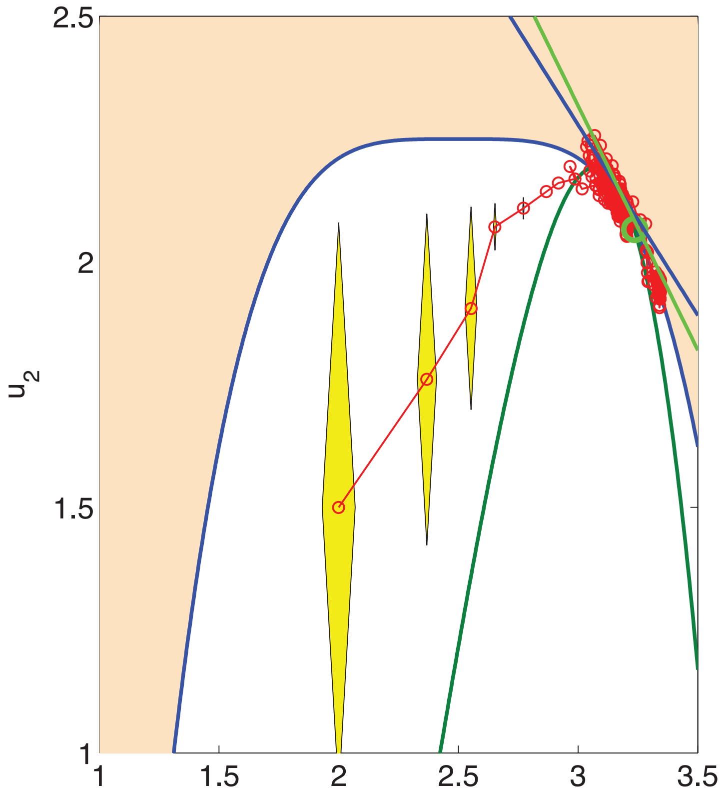
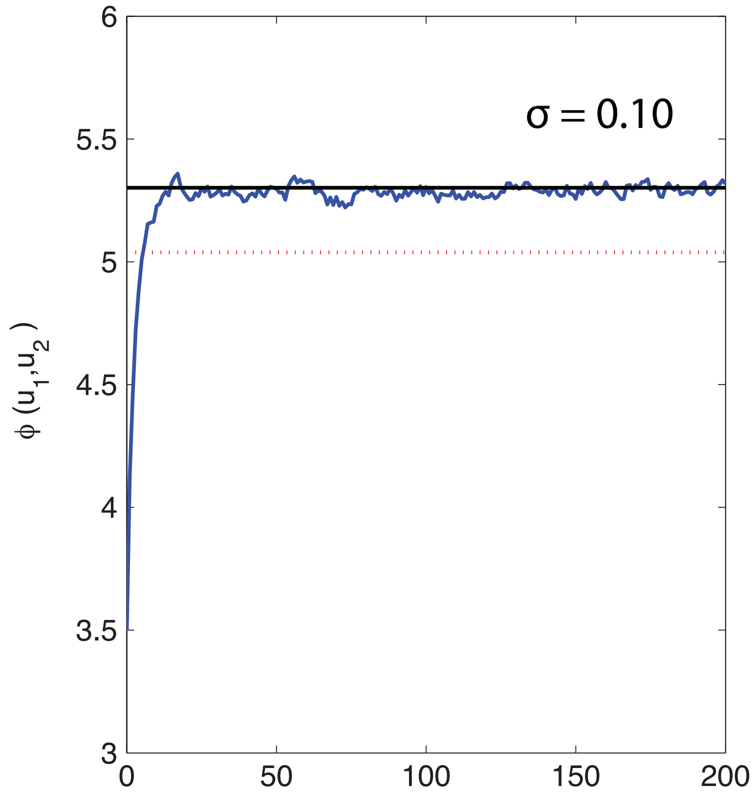


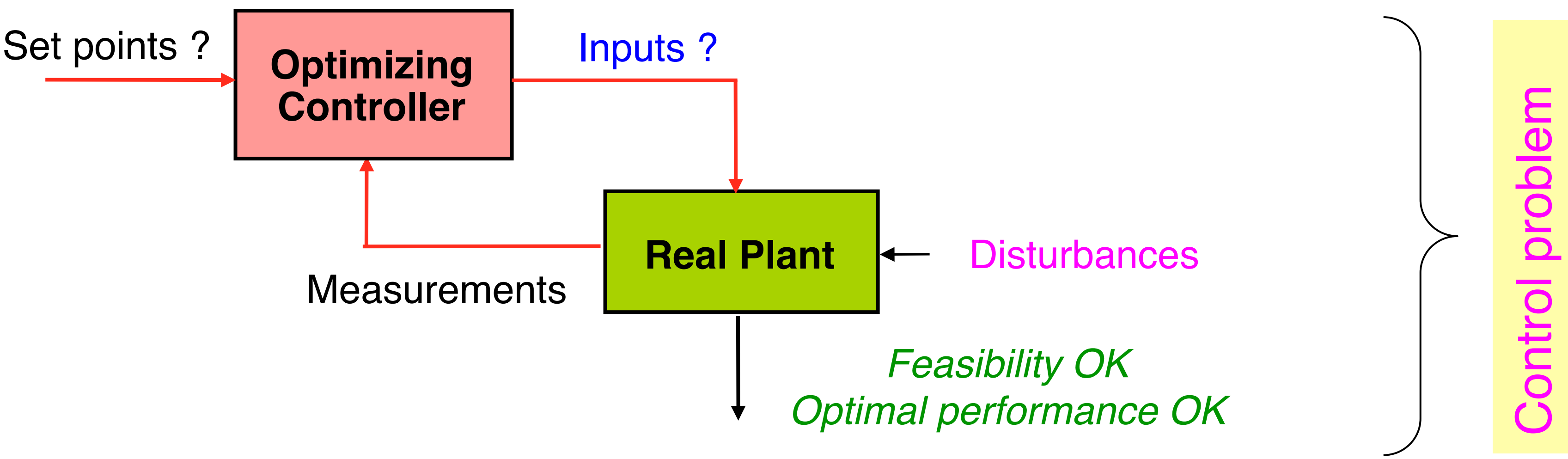


3. Direct Input Adaptation

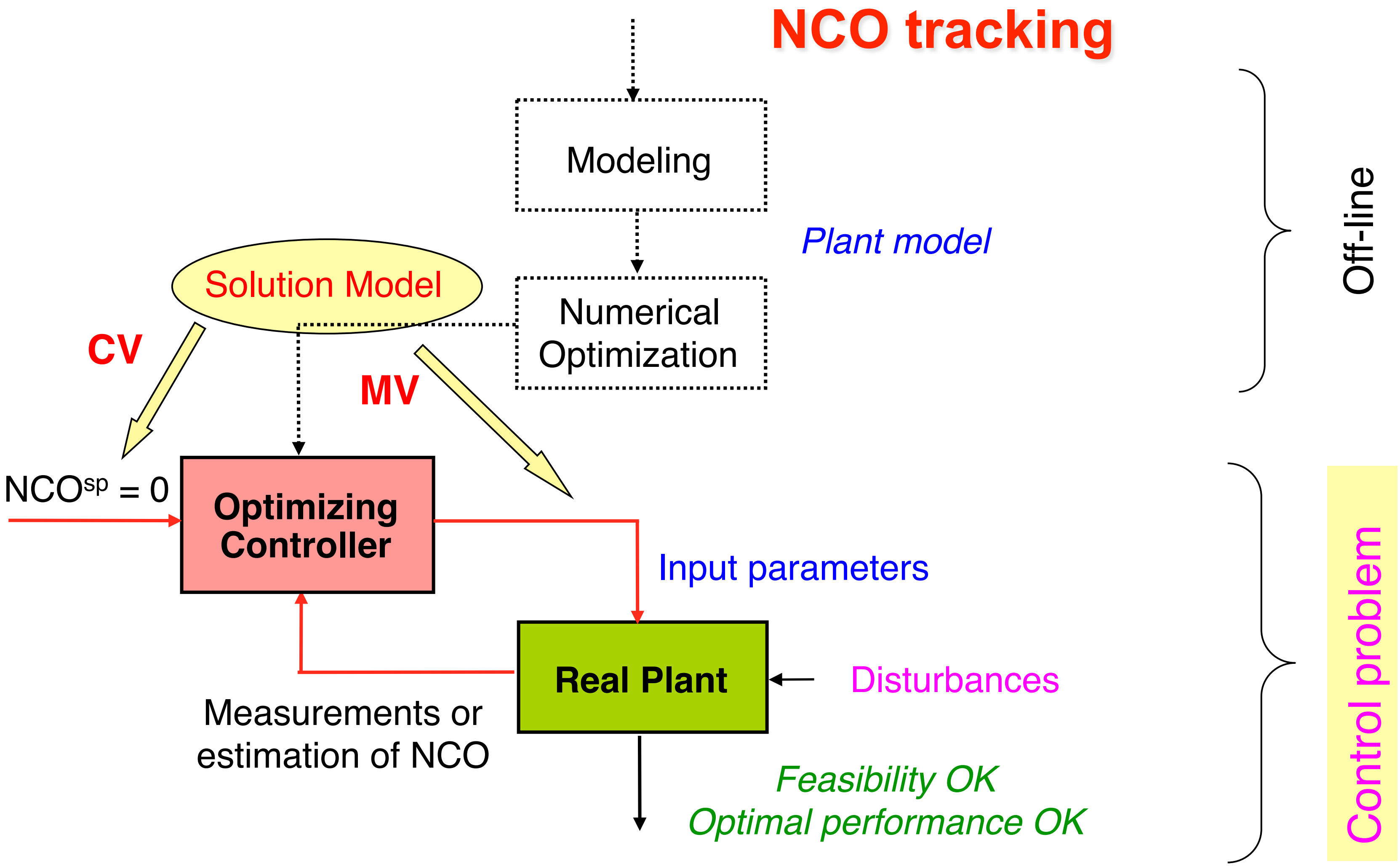
NCO tracking

NCO — **Available degrees of freedom**
Input parameters

CV ? — **MV ?**



3. Direct Input Adaptation



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)

Outline

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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* – Cost and constraint adaptation
- *Adaptation of inputs* – NCO tracking

Application examples

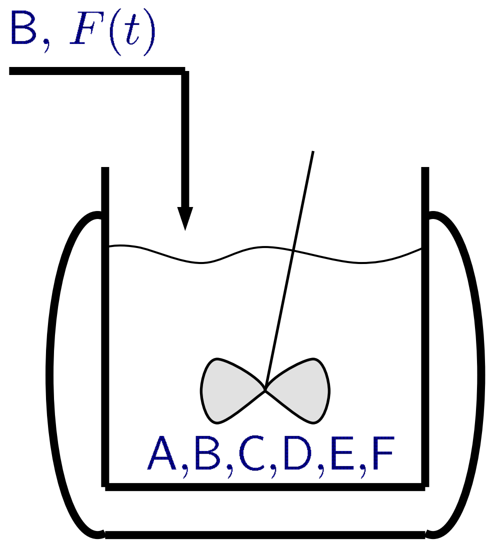
Comparison of Three RTO Schemes

Run-to-Run Optimization of Semi-Batch Reactor

- **Industrial Reaction System** Lonza

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

Simulated Reality *Model*



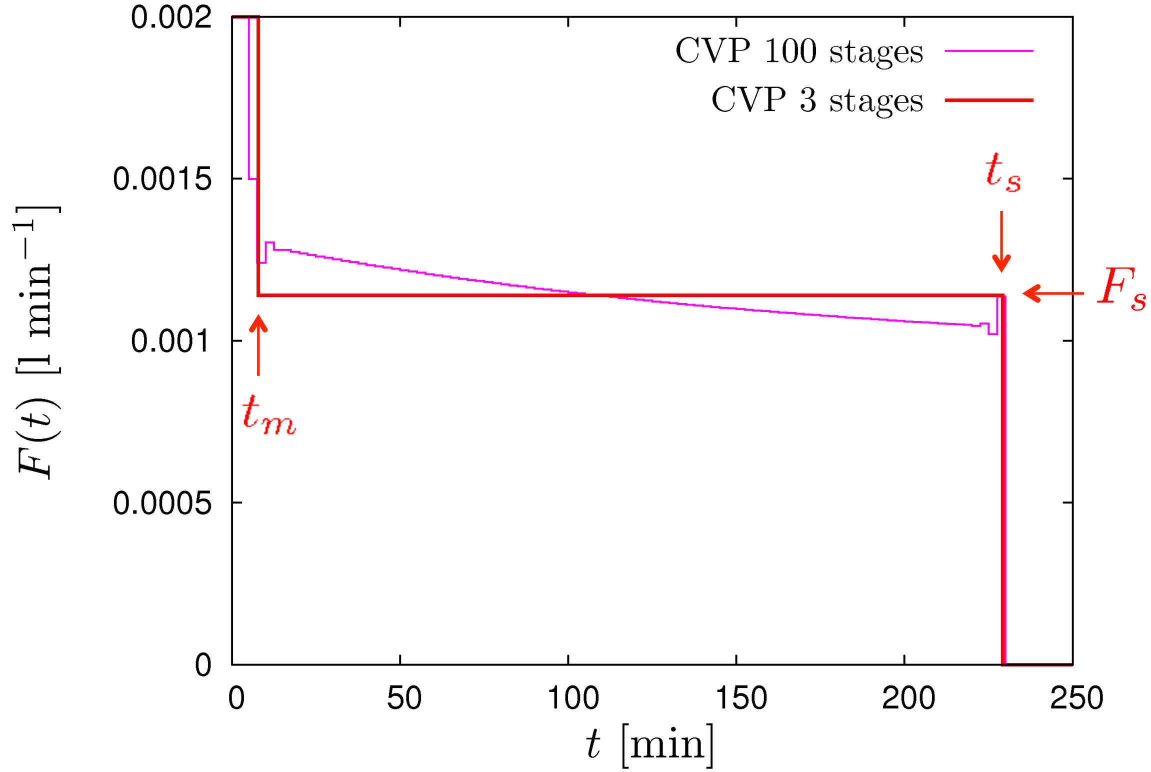
- Manipulated Variables: $F(t)$ (feed flow rate of B)
- Objective: Maximize $n_C(t_f)$ (production of C)
- Constraints:

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

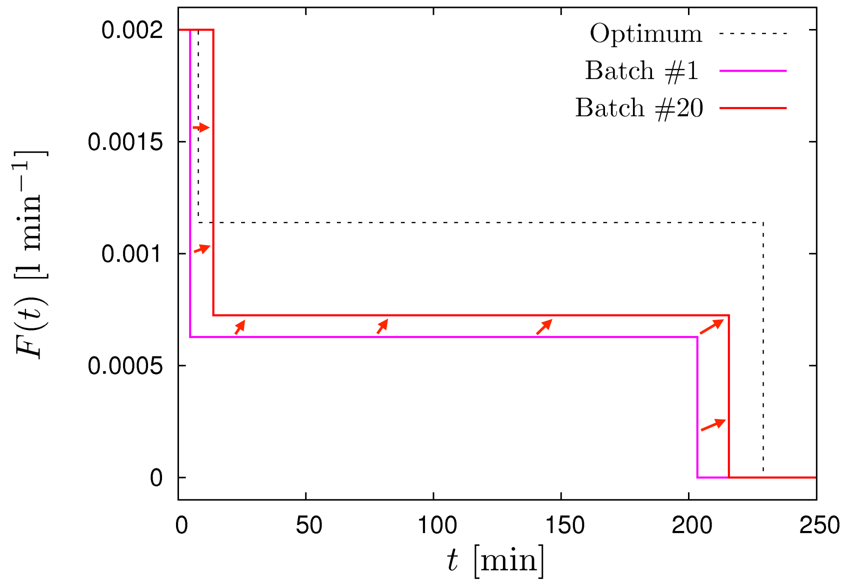
  $J^\star \approx 0.5081$ mol

- **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



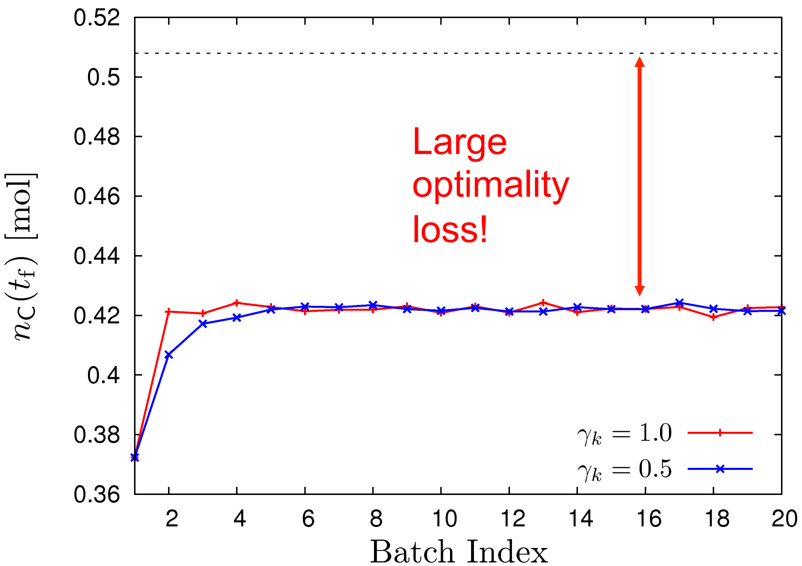
- Measurement Noise: $\sigma_y = 5\%$
  (10% constraint backoffs)

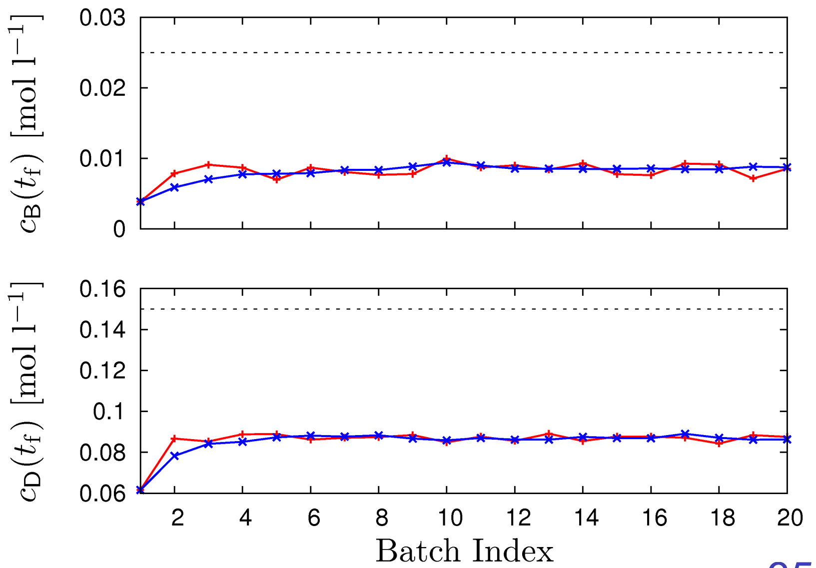
- Identification Objective:

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

- 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 Constraint Modifiers ε_G

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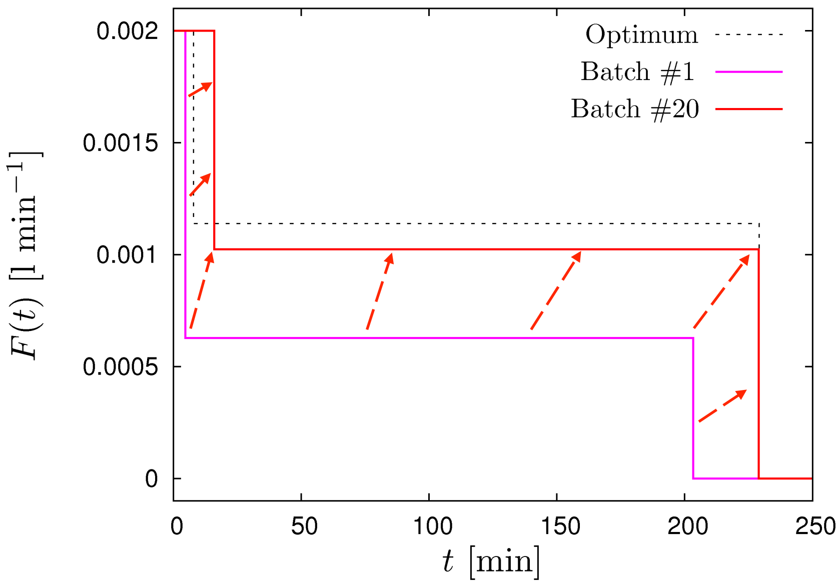
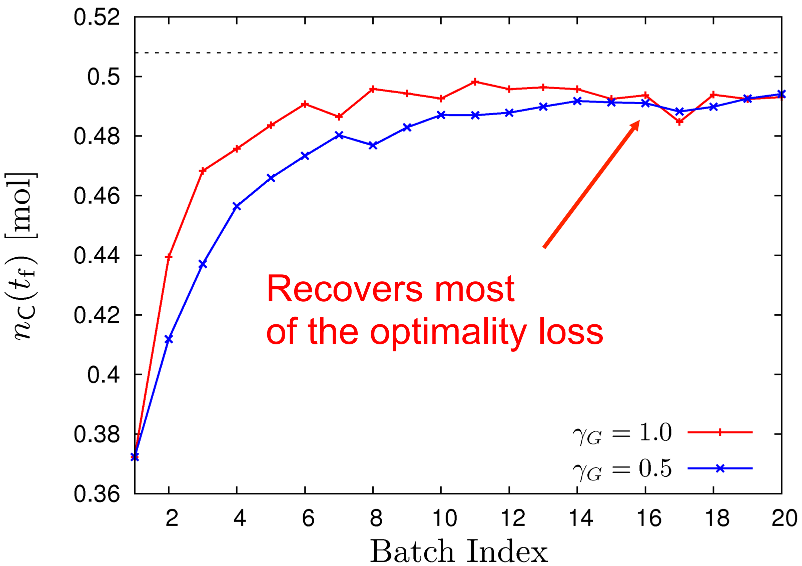
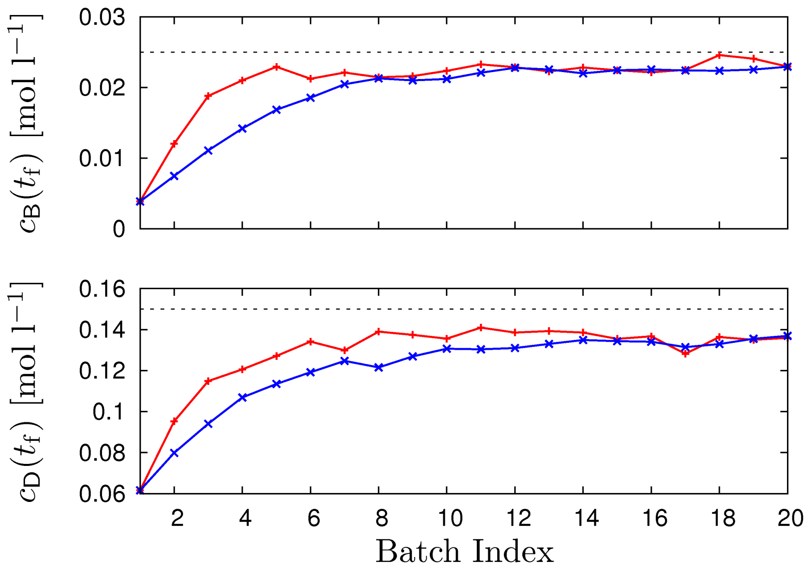


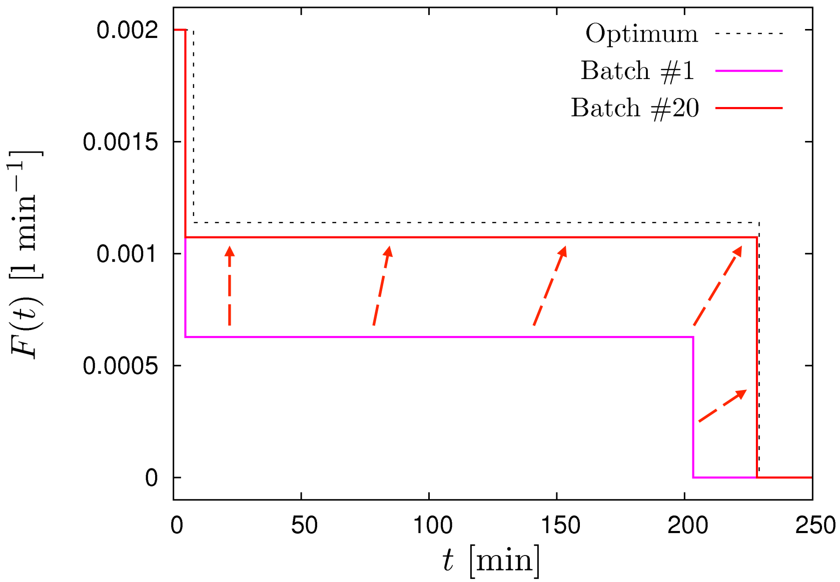
- Measurement Noise: $\sigma_y = 5\%$
  (10% constraint backoffs)
- No Gradient Correction
- Exponential Filter for Modifiers:

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





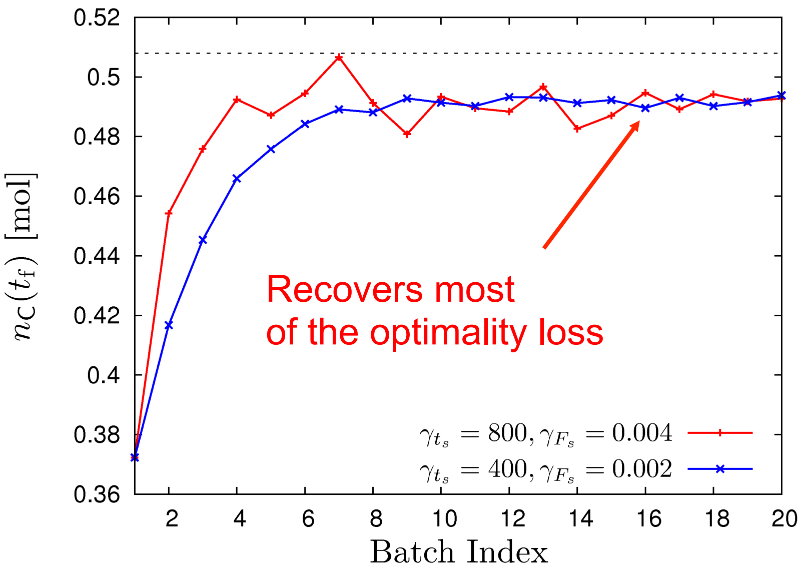
Adaptation of Input Parameters t_s and F_s

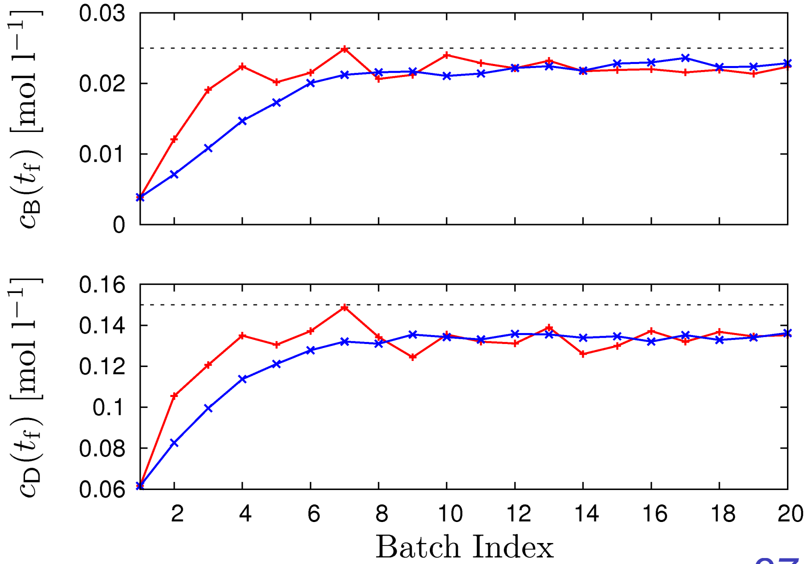


- Measurement Noise: $\sigma_y = 5\%$
  (10% constraint back-offs)
- No Gradient Correction
- Controller Design:

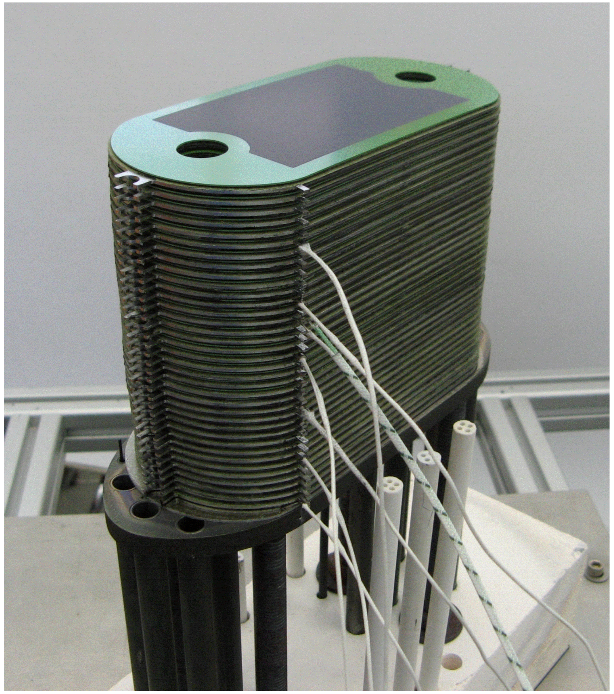
$$t_m = 4.71 \text{ min (fixed)}$$

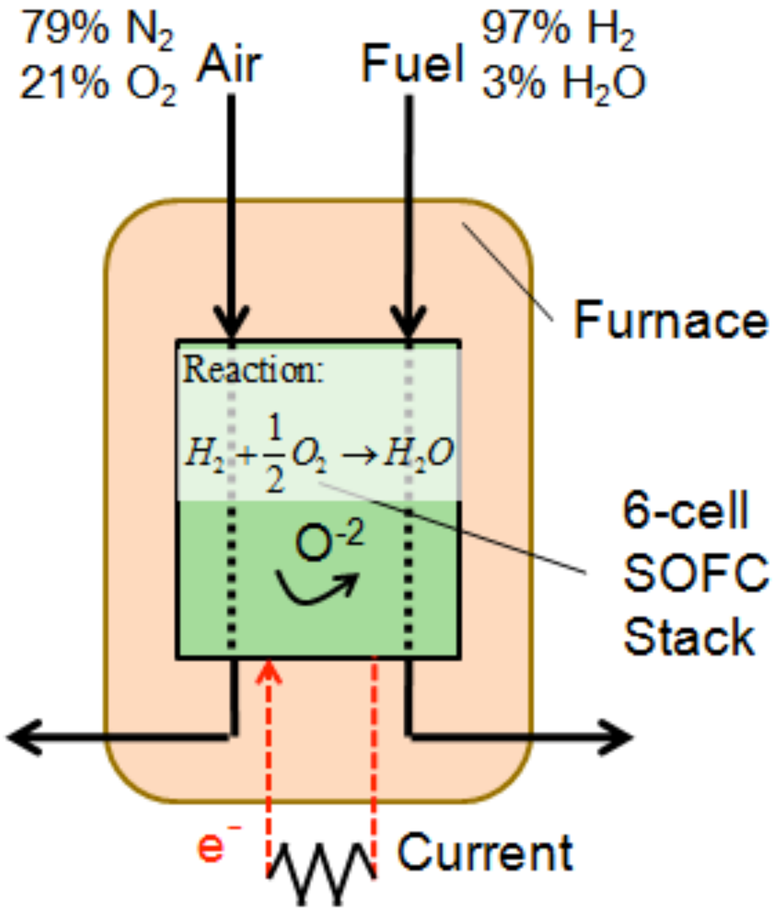
$$\begin{pmatrix} t_s^k \\ F_s^k \end{pmatrix} = \begin{pmatrix} t_s^{k-1} \\ F_s^{k-1} \end{pmatrix} + \begin{pmatrix} \gamma_{t_s} & \\ & \gamma_{F_s} \end{pmatrix} \begin{pmatrix} c_B^{\text{meas}}(t_f) - 0.025 \\ c_D^{\text{meas}}(t_f) - 0.15 \end{pmatrix}_{\pi = \pi^{k-1}}$$





Experimental Solid Oxide Fuel Cell Stack





- Stack of 6 cells, active area of 50 cm^2, metallic interconnector
- Anodes : standard nickel/yttrium stabilized-zirconia (Ni-YSZ)
- Electrolyte : dense YSZ.
- Cathodes: screen-printed (La, Sr)(Co, Fe)O_3
- Operation temperatures between 650 and 850°C.

G.A. Bunin, Z. Wuillemin, 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).

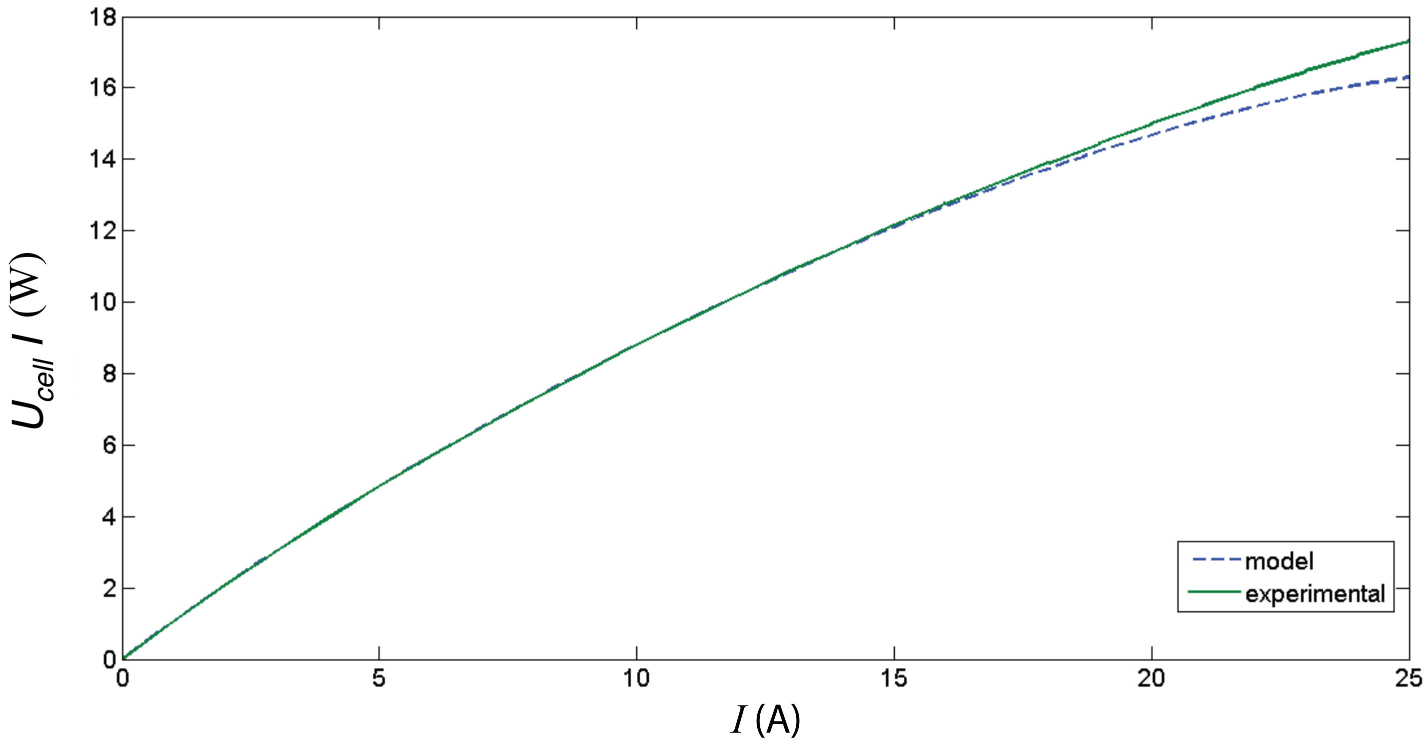
HTceramix SOFCPOWER SOLID OXIDE FUEL CELLS

RTO of SOFC 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 of SOFC via Constraint Adaptation



Challenge: Implement optimal operation with changing power demand

RTO of SOFC via Constraint Adaptation

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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

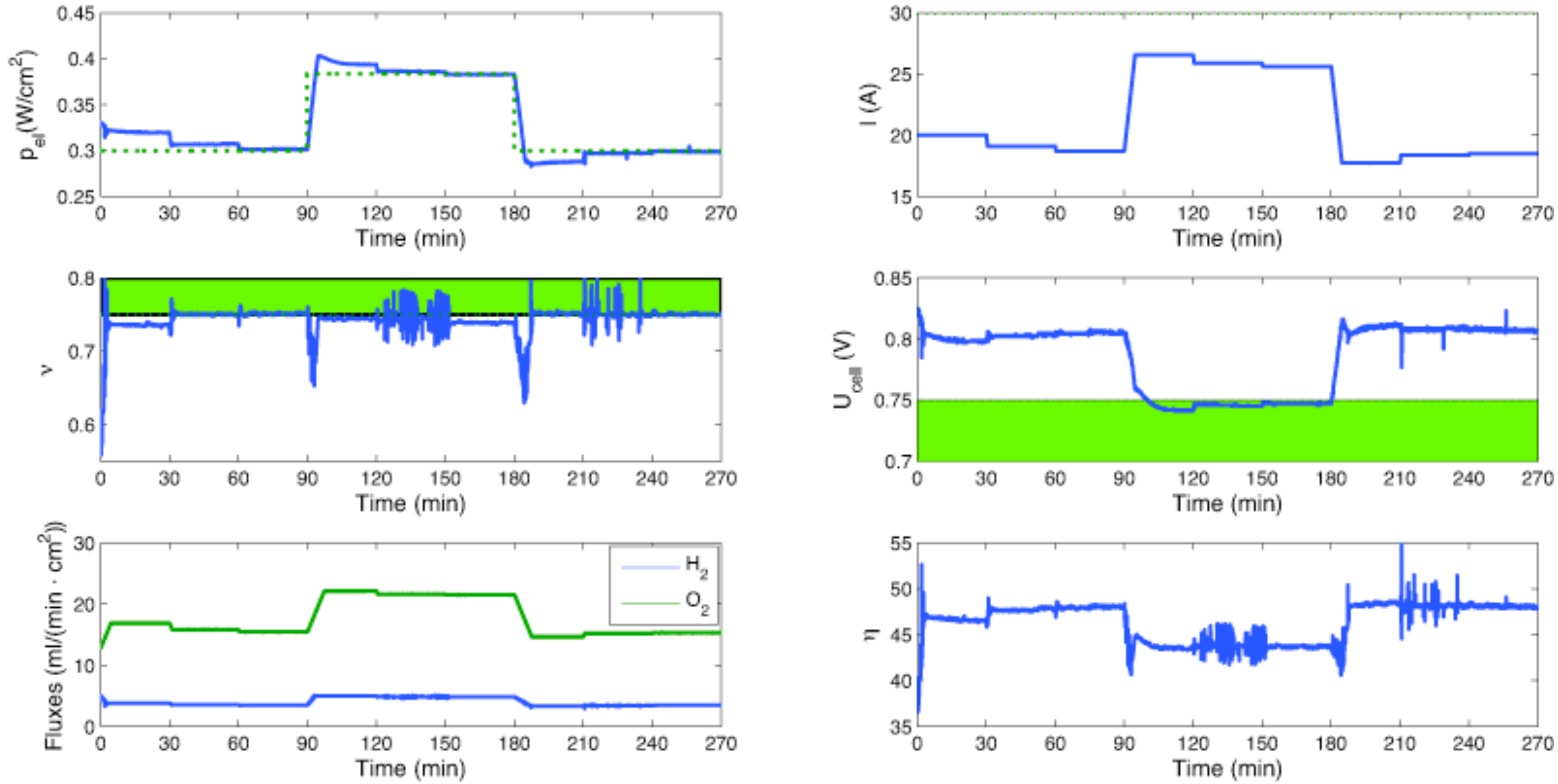
$$
\begin{aligned}
\max_{u_k} \quad & \eta(\mathbf{u}_k, \mathbf{\Theta}) \\
\text{s.t.} \quad & p_{\text{el}}(\mathbf{u}_k, \mathbf{\Theta}) + \varepsilon_{k-1}^{p_{\text{el}}} = p_{el}^{S} \\
& U_{\text{cell}}(\mathbf{u}_k, \mathbf{\Theta}) + \varepsilon_{k-1}^{U_{\text{cell}}} \geq 0.75V \\
& \nu(\mathbf{u}_k) \leq 0.75 \\
& 4 \leq 2\frac{u_{2,k}}{u_{1,k}} = \lambda_{air}(\mathbf{u}_k) \leq 7 \\
& u_{1,k} \geq 3.14\,\text{mL/(min cm}^2) \\
& u_{3,k} \leq 30\,\text{A}
\end{aligned}
$$

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

$$
\begin{aligned}
\varepsilon_k^{p_{\text{el}}} &= \left(1\text{-}K_{p_{\text{el}}}\right)\varepsilon_{k-1}^{p_{\text{el}}} + K_{p_{\text{el}}}\left[p_{\text{el,p,k}} - p_{\text{el}}(\mathbf{u}_k, \mathbf{\Theta})\right] \\
\varepsilon_k^{U_{\text{cell}}} &= \left(1\text{-}K_{U_{\text{cell}}}\right)\varepsilon_{k-1}^{U_{\text{cell}}} + K_{U_{\text{cell}}}\left[U_{\text{cell,p,k}} - U_{\text{cell}}(\mathbf{u}_k, \mathbf{\Theta})\right]
\end{aligned}
$$

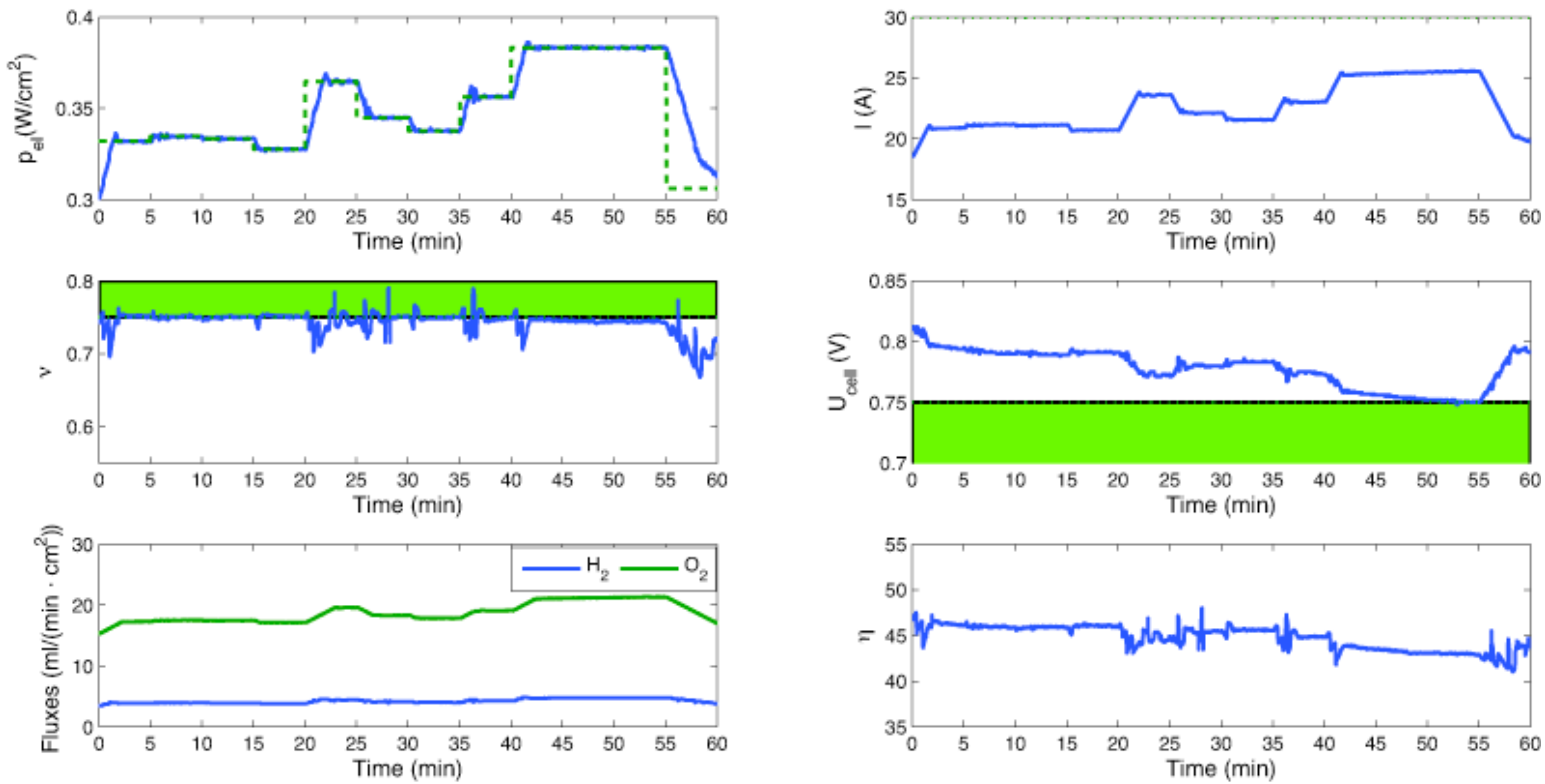
Slow RTO ("Wait for Steady State")

- 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



Conclusions

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- All models are wrong, but some are useful (G.E.P. Box, 1979)
  - Model is not the truth, but rather a tool
  - Modeling for optimization
  - Use measurements for process improvement
  - What is the best handle for (model) correction?

- Intuitive "repeated identification and optimization" suffers from lack of model adequacy
- Importance of being able to measure/estimate the plant KKT conditions
- Results for RTO extend to DRTO
  - Role of the model in two-step approaches?
  - Role of the model in MPC?
  - Estimation of states with inaccurate model?
  - Is model adequacy ensured?