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Real-time optimization of a solid-oxide electrolyser

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Partnership

reactt

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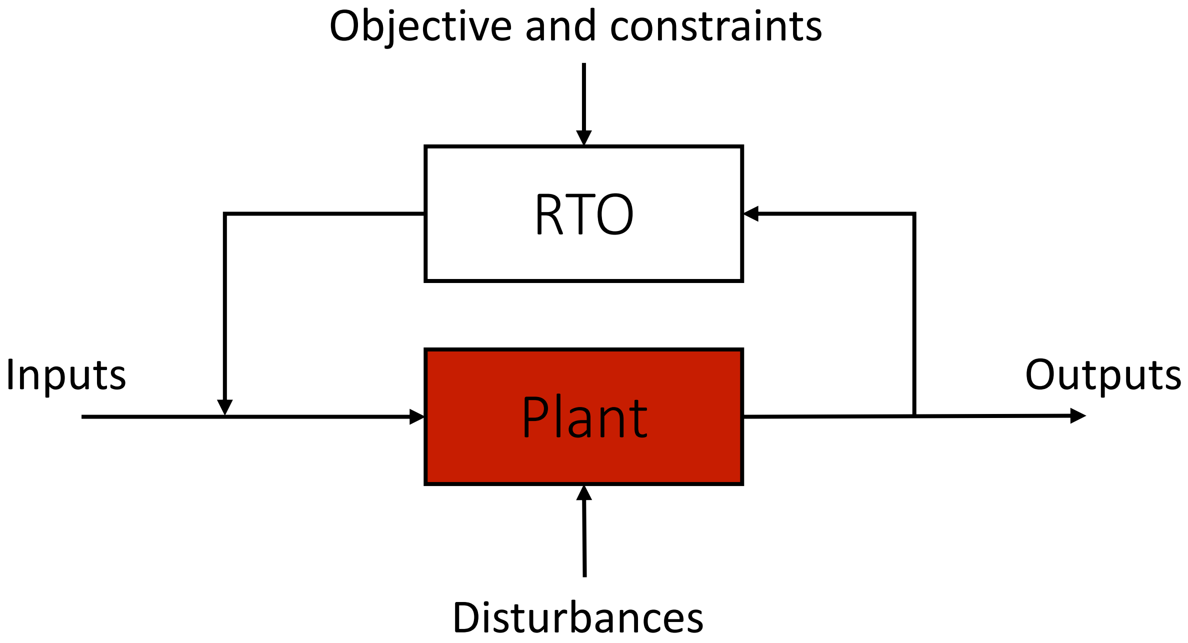
Real-Time Optimization

Techniques that use process measurements to improve plant performance in the presence of

- Disturbances
- Plant-model mismatch



Static Real-Time Optimization

- Adaptation of cost and constraint functions – **Modifier adaptation**

Model Adequacy Conditions

Definition 1 (Model-adequacy criterion). *A process model is said to be adequate for use in an RTO scheme if it is capable of producing a fixed point that is a local minimum for the RTO problem at the plant optimum* $\mathbf{u}_p^*$.

Proposition 1 (Model-adequacy conditions for MA). *Let* $\mathbf{u}_p^*$ *be a regular point for the constraints and the unique plant optimum. Let* $\nabla_r^2\mathcal{L}(\mathbf{u}_p^*)$ *denote the reduced Hessian of the Lagrangian of the optimization problem at* $\mathbf{u}_p^*$. *Then, the following statements hold:*

i. if $\nabla_r^2\mathcal{L}(\mathbf{u}_p^*)$ *is positive definite, then the process model is adequate for use in the MA scheme.*

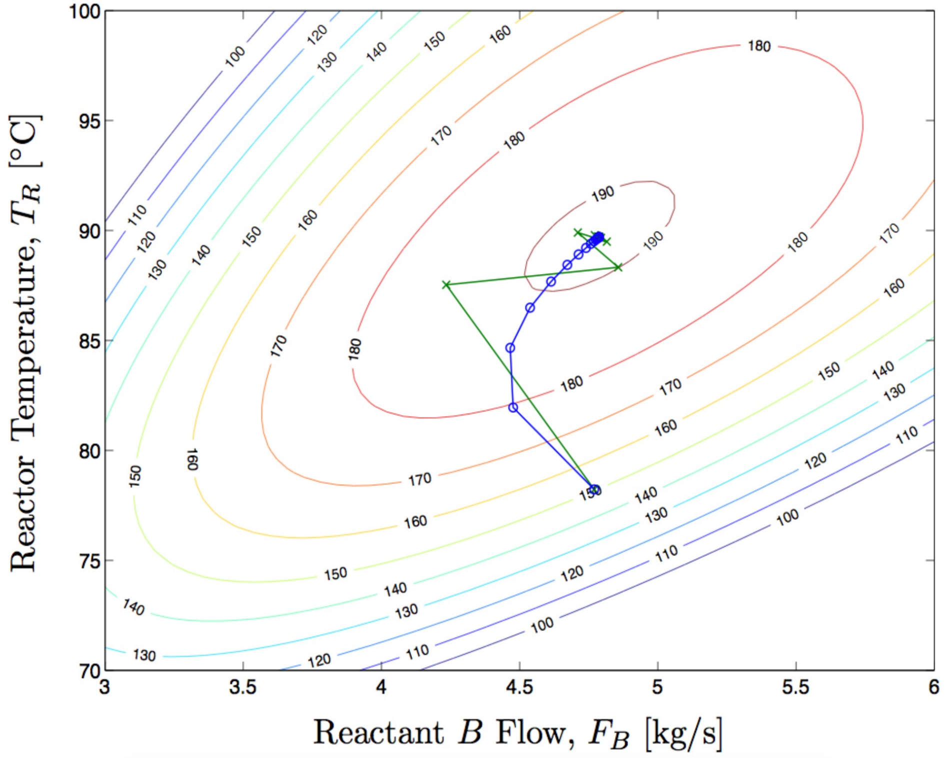
ii. If $\nabla_r^2\mathcal{L}(\mathbf{u}_p^*)$ *is not positive semi-definite, then the process model is inadequate for use in the MA scheme.*

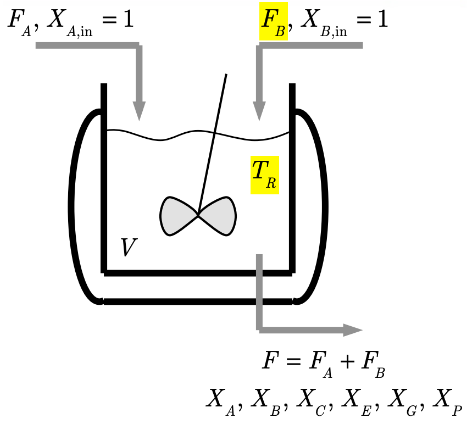
iii. If $\nabla_r^2\mathcal{L}(\mathbf{u}_p^*)$ *is positive semi-definite and singular, then the second-order conditions are not conclusive with respect to model adequacy.*

Marchetti, Alejandro G., Grégory François, Timm Faulwasser, and Dominique Bonvin. "Modifier adaptation for real-time optimization—methods and applications." Processes 4, no. 4 (2016): 55.

KKT Matching

Theorem 1 (MA convergence) KKT matching. *Consider the problem of optimizing a plant with an inaccurate yet adequate model using MA, let* $\mathbf{u}_\infty = \lim_{k\to\infty} \mathbf{u}_k$ *be a fixed point of the MA iterative scheme. Then, not only* $\mathbf{u}_\infty$ *is a KKT point of the modified model-based optimization Problem (1),* $\mathbf{u}_k$ *is also a KKT point of the plant problem.*





Williams-Otto Reactor

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

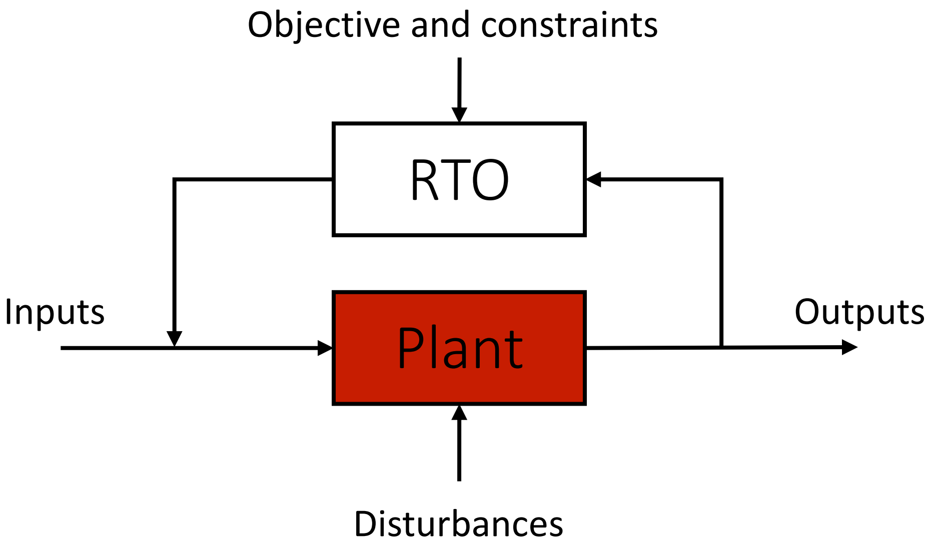
Converges to plant optimum!

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

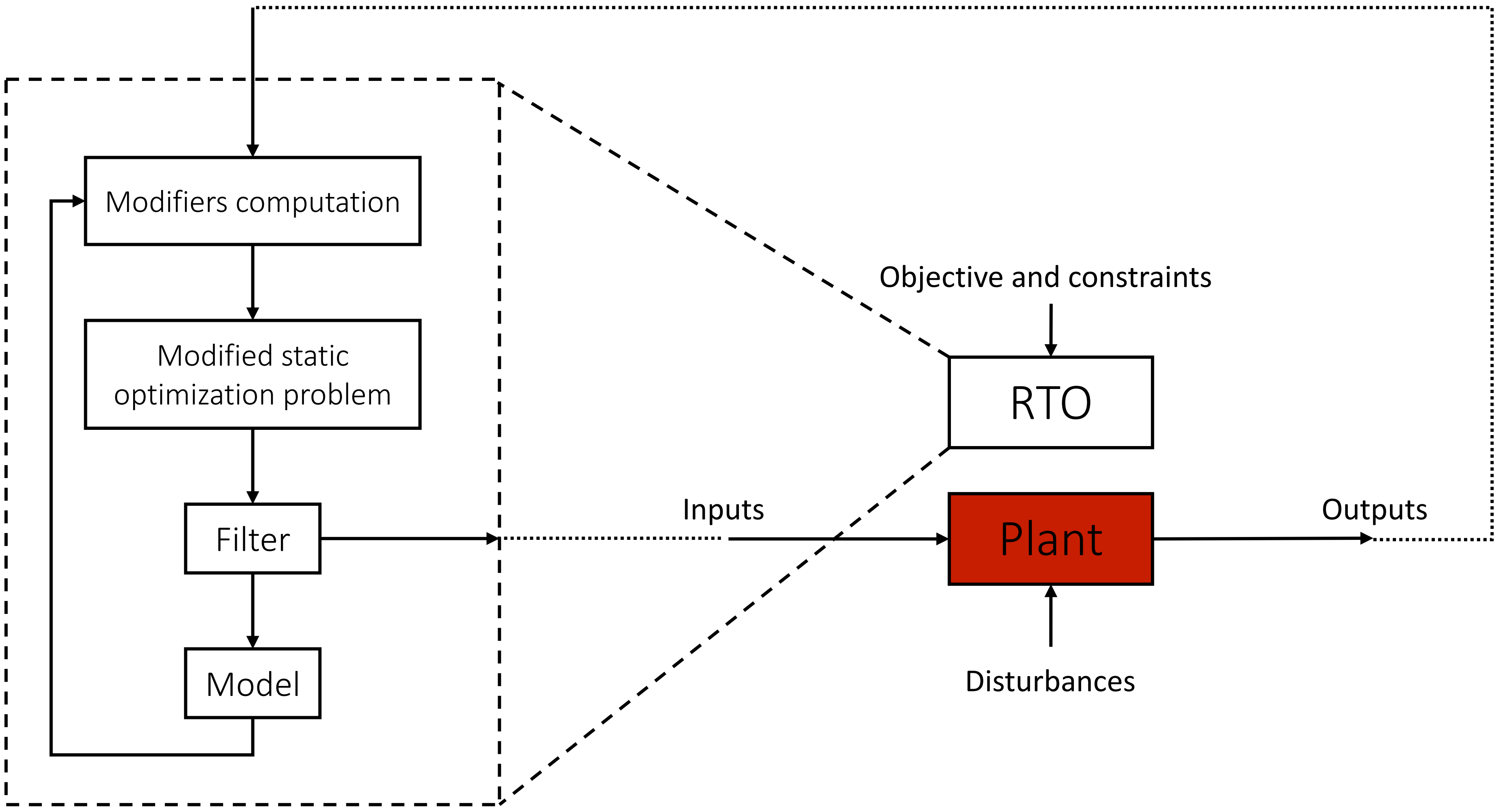
Real-time optimization

- Introduces measurements into the optimization scheme
- Optimization with its requirements is performed iteratively
- Reaches optimal conditions
- Reaching the set electric power/hydrogen production requires more than just manipulate current if done optimally
- Multiple efficiencies for a set electric power/hydrogen production
- Optimal way of changing the operating conditions
- Ensures the set of the electric power/hydrogen production even if the system did not set to steady-state
- Deals with degrading systems: feasible operation
- Delays and slows down degradation

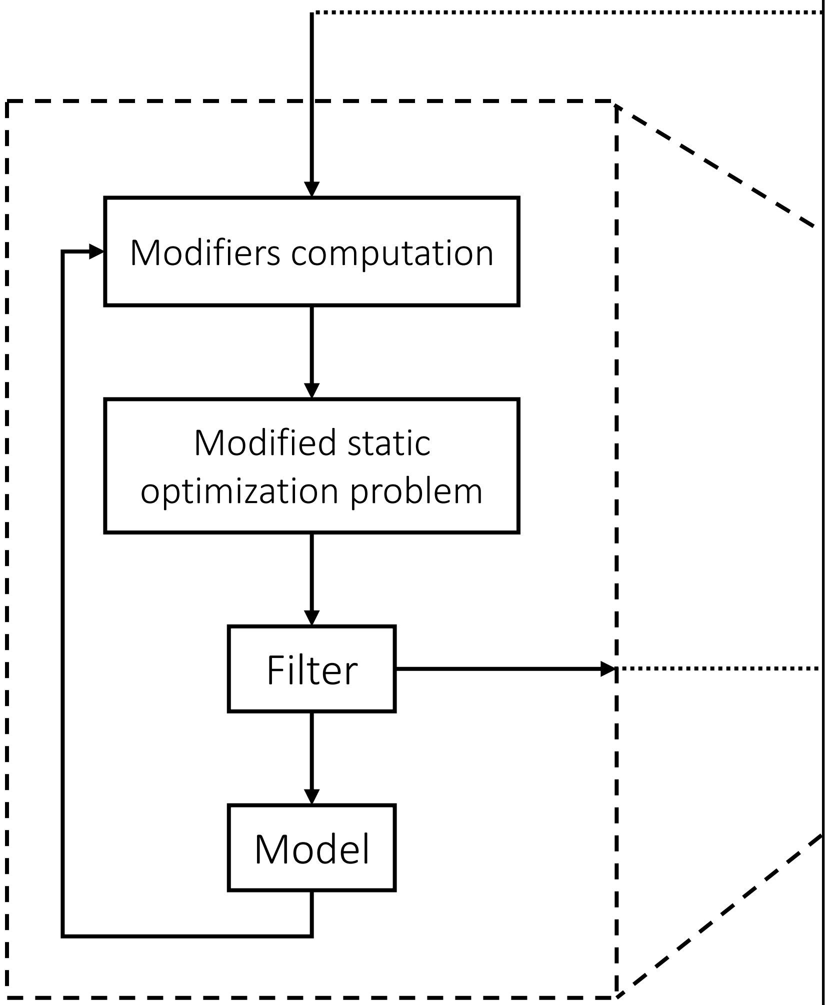
Real-time optimization scheme



Real-time optimization scheme



Real-time optimization scheme



Main Idea

$$
\begin{aligned}
\mathbf{u}^\star_{k+1} = \arg\min_{u} \quad & \Phi(\mathbf{u}) \\
\text{s.t.} \quad & \mathbf{H}(\mathbf{u}) + \hat{\boldsymbol{\epsilon}}_j^{\mathbf{H}} = \mathbf{0} \\
& \mathbf{G}(\mathbf{u}) + \hat{\boldsymbol{\epsilon}}_j^{\mathbf{G}} \leq \mathbf{0} \\
& \mathbf{u}^L \leq \mathbf{u} \leq \mathbf{u}^U
\end{aligned}
$$

$$
\begin{aligned}
\text{with:} \quad \hat{\boldsymbol{\epsilon}}_j^{\mathbf{H}} &:= \mathbf{H}_p^{dyn}(t_j) - \mathbf{H}^{dyn}(t_j) \\
\hat{\boldsymbol{\epsilon}}_j^{\mathbf{G}} &:= \mathbf{G}_p^{dyn}(t_j) - \mathbf{G}^{dyn}(t_j)
\end{aligned}
$$

Dynamic Model:

$$
\begin{aligned}
\dot{\mathbf{x}}(t) &= \mathbf{f}\left(\mathbf{x}(t),\ \mathbf{u}(t), \boldsymbol{\theta}\right), \quad \mathbf{x}(0) = \mathbf{x}_0 \\
\mathbf{y}(t) &= \mathbf{F}\left(\mathbf{x}(t),\ \mathbf{u}(t), \boldsymbol{\theta}\right)
\end{aligned}
$$

where:

$$
\begin{aligned}
\mathbf{H}^{dyn}(t_j) &:= \ \mathbf{h}\big(\mathbf{u}_j, \mathbf{y}(t_j)\big) \\
\mathbf{G}^{dyn}(t_j) &:= \ \mathbf{g}\big(\mathbf{u}_j, \mathbf{y}(t_j)\big)
\end{aligned}
$$

Real-time optimization scheme

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Main features

- Add bias correction terms to the constraints
- Works well when the optimum is mainly determined by active constraints
- Upon convergence, it converges to feasible point
- Converges to a KKT of the plant if model adequacy is satisfied
- Fast convergence

Main Idea

$$\begin{aligned} \mathbf{u}_{k+1}^{\star} = \arg\min_{u} \quad & \Phi(\mathbf{u}) \\ \text{s.t.} \quad & \mathbf{H}(\mathbf{u}) + \hat{\boldsymbol{\epsilon}}_j^{\mathbf{H}} = \mathbf{0} \\ & \mathbf{G}(\mathbf{u}) + \hat{\boldsymbol{\epsilon}}_j^{\mathbf{G}} \leq \mathbf{0} \\ & \mathbf{u}^L \leq \mathbf{u} \leq \mathbf{u}^U \end{aligned}$$

$$\begin{aligned} \text{with:} \quad \hat{\boldsymbol{\epsilon}}_j^{\mathbf{H}} &:= \mathbf{H}_p^{dyn}(t_j) - \mathbf{H}^{dyn}(t_j) \\ \hat{\boldsymbol{\epsilon}}_j^{\mathbf{G}} &:= \mathbf{G}_p^{dyn}(t_j) - \mathbf{G}^{dyn}(t_j) \end{aligned}$$

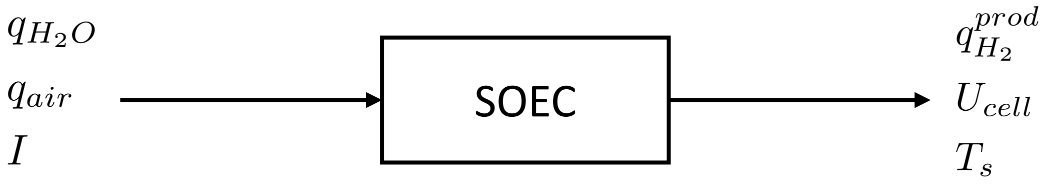
Dynamic Model:

$$\begin{aligned} \dot{\mathbf{x}}(t) &= \mathbf{f}\left(\mathbf{x}(t),\ \mathbf{u}(t), \boldsymbol{\theta}\right), \quad \mathbf{x}(0) = \mathbf{x}_0 \\ \mathbf{y}(t) &= \mathbf{F}\left(\mathbf{x}(t),\ \mathbf{u}(t), \boldsymbol{\theta}\right) \end{aligned}$$

where:

$$\begin{aligned} \mathbf{H}^{dyn}(t_j) &:= \ \mathbf{h}\big(\mathbf{u}_j, \mathbf{y}(t_j)\big) \\ \mathbf{G}^{dyn}(t_j) &:= \ \mathbf{g}\big(\mathbf{u}_j, \mathbf{y}(t_j)\big) \end{aligned}$$

Real-time optimization of an SOE stack



- The optimization approach is solved together with the tendency model
- The SOE model itself is not updated
- Here only the constraint functions are modified by using simultaneously measurements from the tendency model and the SOE stack and the tendency model

$$\mathbf{u} = \arg\max_{\mathbf{u}} \ \eta_{el} = \frac{q_{H_2} LVH_{H_2}}{P_{el}}$$

$$\begin{aligned} \text{s.t} \quad & q_{H_2}^{prod} = q_{H_2}^{prod,S} + \varepsilon_{q_{H_2}} \quad \text{NL.min}^{-1} \\ & 680 \leq T_{stack} + \varepsilon_{T_{stack}} \leq 780\ ^{\circ}\text{C} \\ & 1.3 \leq U_{cell} + \varepsilon_{U_{cell}} \leq 1.4\ \text{V} \\ & FU \leq 0.9 \\ & q_{air} \leq 150\ \text{NL.min}^{-1} \end{aligned}$$

Stack energy balance

$$\rho_s V_s C_{p,s} \frac{dT_s}{dt} = \sum_{in} q_{in,i} H_{in,i}(T_{in,i}) - \sum_{out} q_{out,i} H_{out,i}(T_s) - Pel - Q_{loss}$$

Cell voltage (electrochemistry)

$$U_{cell} = U_N + \eta_{act} + \eta_{ohm} + \eta_{conc}$$

$$\boldsymbol{P_{el} = U_{cell} N_{cell} I}$$

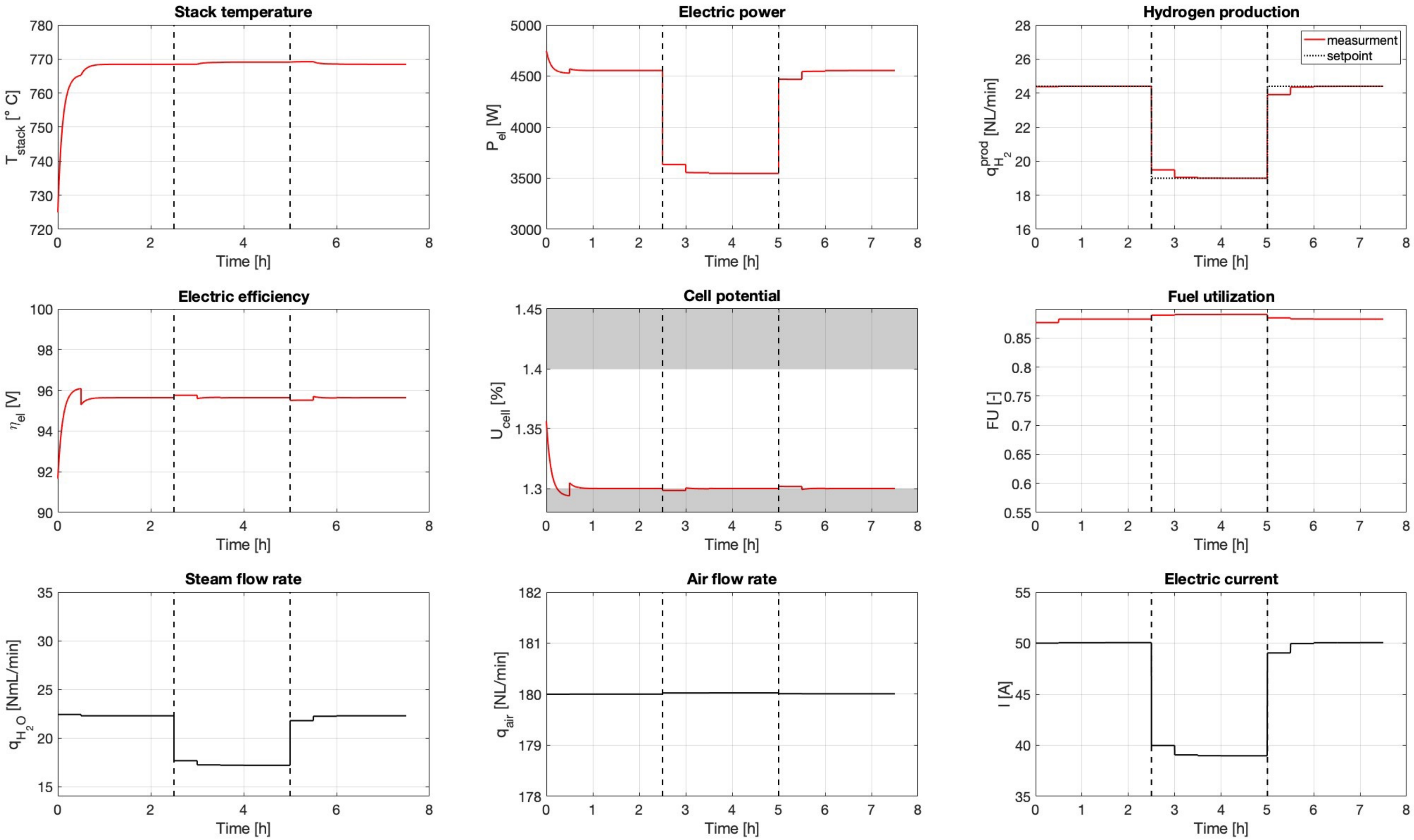
Material balance

$$\begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} M_{A0} - M_A \\ M_{B0} - M_B \\ M_{C0} - M_C \\ M_{D0} - M_D \\ M_{E0} - M_E \\ M_{F0} - M_F \end{bmatrix} + \begin{bmatrix} -1 & -1 \\ -1 & 0 \\ +1 & -1 \\ +1 & 0 \\ 0 & +1 \\ 0 & +1 \end{bmatrix} \begin{bmatrix} \xi_1 \\ \xi_2 \end{bmatrix} = 0$$

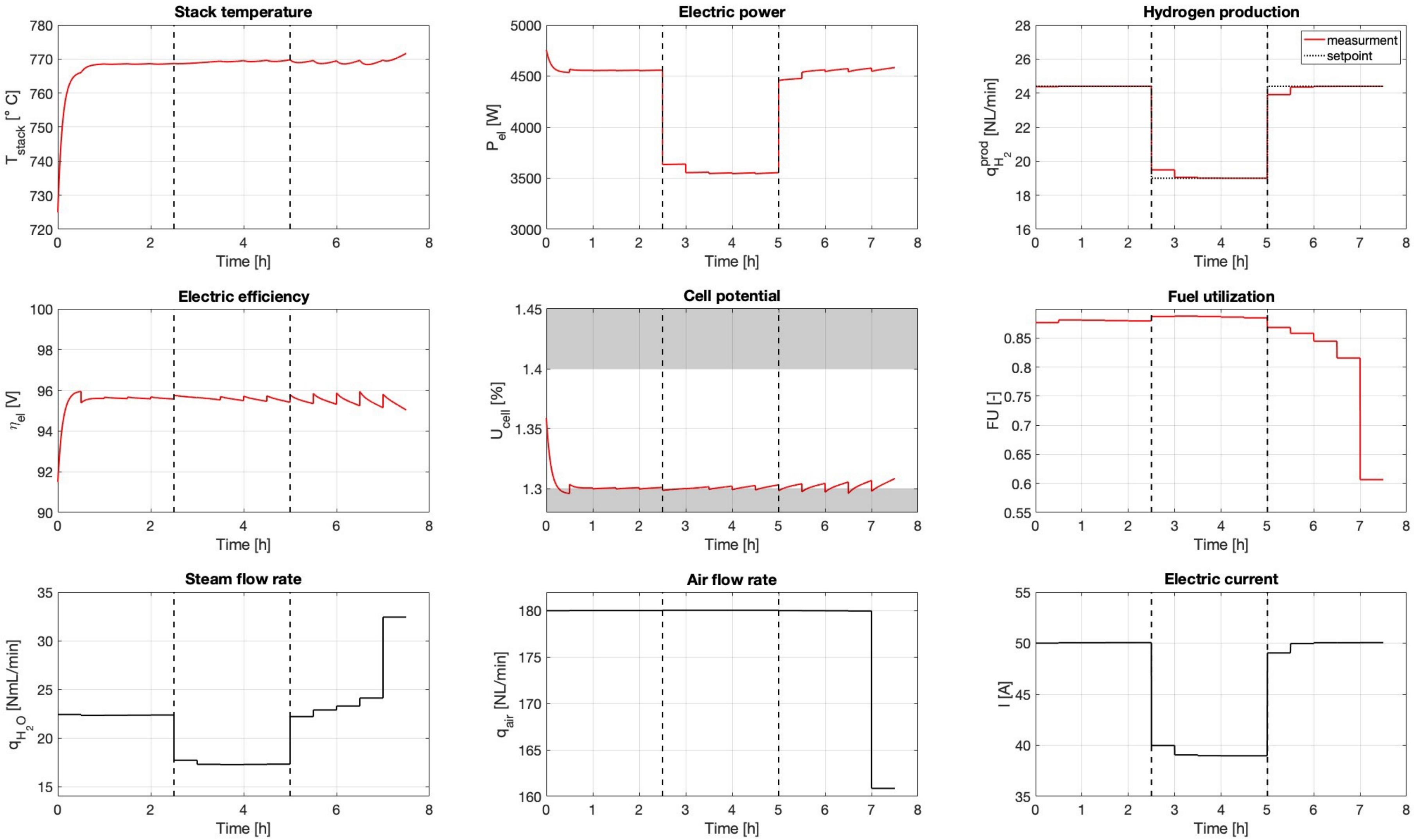
Hydrogen production setpoint

$$q_{H_2}^{prod,S}(t) = \begin{cases} 24.4\ [NL/min], & \text{t} \leq 2.5\ \text{h} \\ 19\ [NL/min], & 2.5\ \text{h} < \text{t} \leq 10\ \text{h} \\ 24.4\ [NL/min], & \text{t} > 10\ \text{h}. \end{cases}$$

Simulation results of RTO applied to an SOEC



Simulation results of RTO applied to a SOEC with induced degradation



Conclusions

- RTO is a family of optimization methods that incorporate process measurements in the optimization framework to drive a real process to optimal performance despite disturbance

- Our group in HES-SO develops RTO approaches that tackle specific targets defined by industry requirements as well as proving their properties and experimental application for validation

- RTO is suited for a broad range of industrial processes, including electrolysers and fuel-cell systems

- The main features of RTO includes the ability of reaching plant optimality and constraint satisfaction

- A variant of modifier-adaptation has been developed and applied to a commercial system (SOLIDpower) and an ethanol-fed SOFC system

Acknowledgement

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