Enforcing optimal operation of FCS despite degradation via real-time optimization

Tafarel de Avila Ferreira

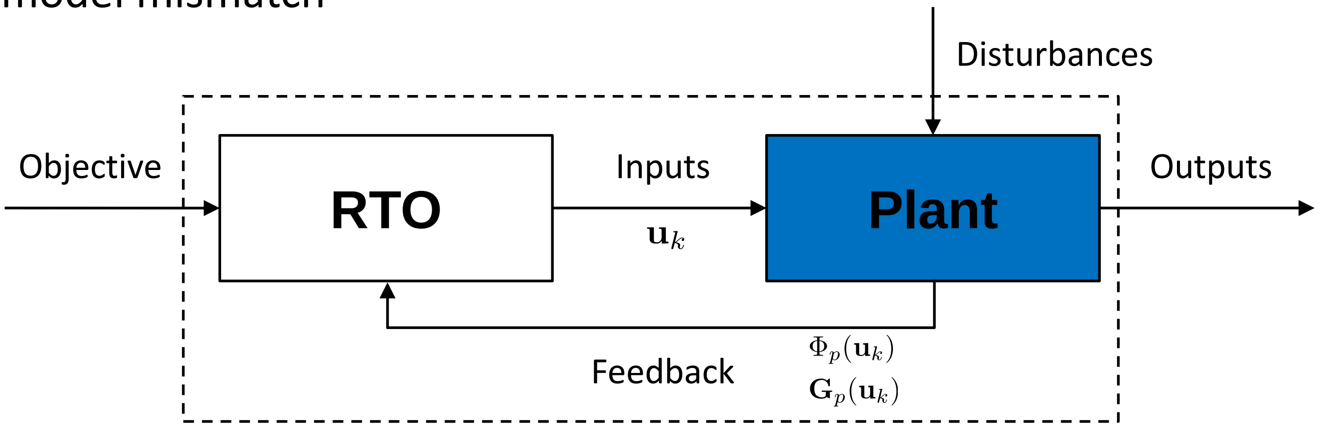
Workshop – From basic to applied research towards durable and reliable fuel cells

July 5th, 2022
Lucerne, Switzerland

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**

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The Role of Model in RTO

Plant

$$\begin{aligned}\min_{\mathbf{u}} \quad & \Phi_p(\mathbf{u}) := \phi(\mathbf{u}, \mathbf{y}_p(\mathbf{u})) \\ \text{s.t.} \quad & G_{p,i}(\mathbf{u}) := g_i(\mathbf{u}, \mathbf{y}_p(\mathbf{u})) \leq 0 \\ & i = 1, \ldots, n_g \\ & \mathbf{u} \in \mathcal{U}\end{aligned}$$

Model

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Challenge

- **Optimal plant** operation!
- **Uncertain** model, i.e. $\phi_p(u) \neq \phi(u, \theta)$, $G_{p,i}(u) \neq G_i(u, \theta)$.

Real-Time Optimization

- Use process measurements
- Which entities should be measured?
- How should these measurements be used?

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The Role of Model in RTO

Plant

Model

$$
\begin{aligned}
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\end{aligned}
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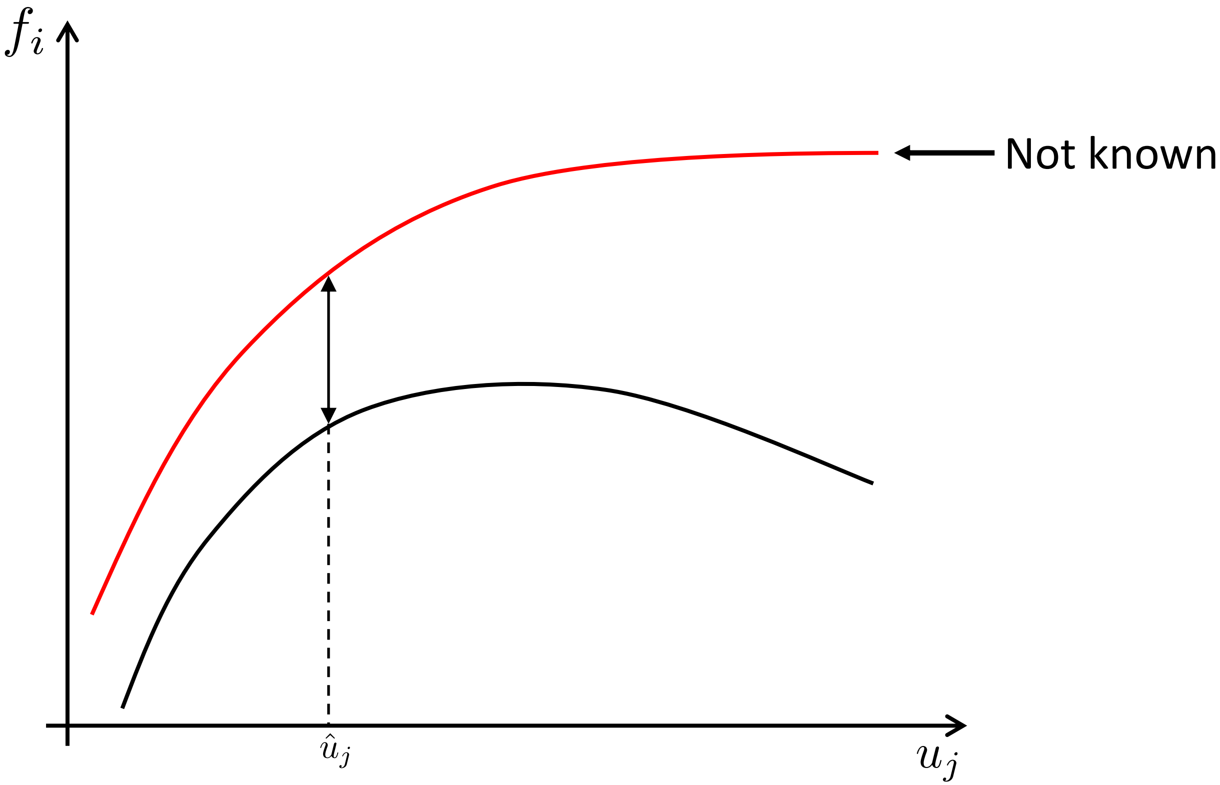
SOLIDpower. https:www.solidpower.com. Accessed 1 July 2022.

Basic Features of Modifier Adaptation

How is the optimization scheme adapted?

Modifier Adaptation: Zeroth- and first-order correction terms added to cost and constraint functions to the optimization problem



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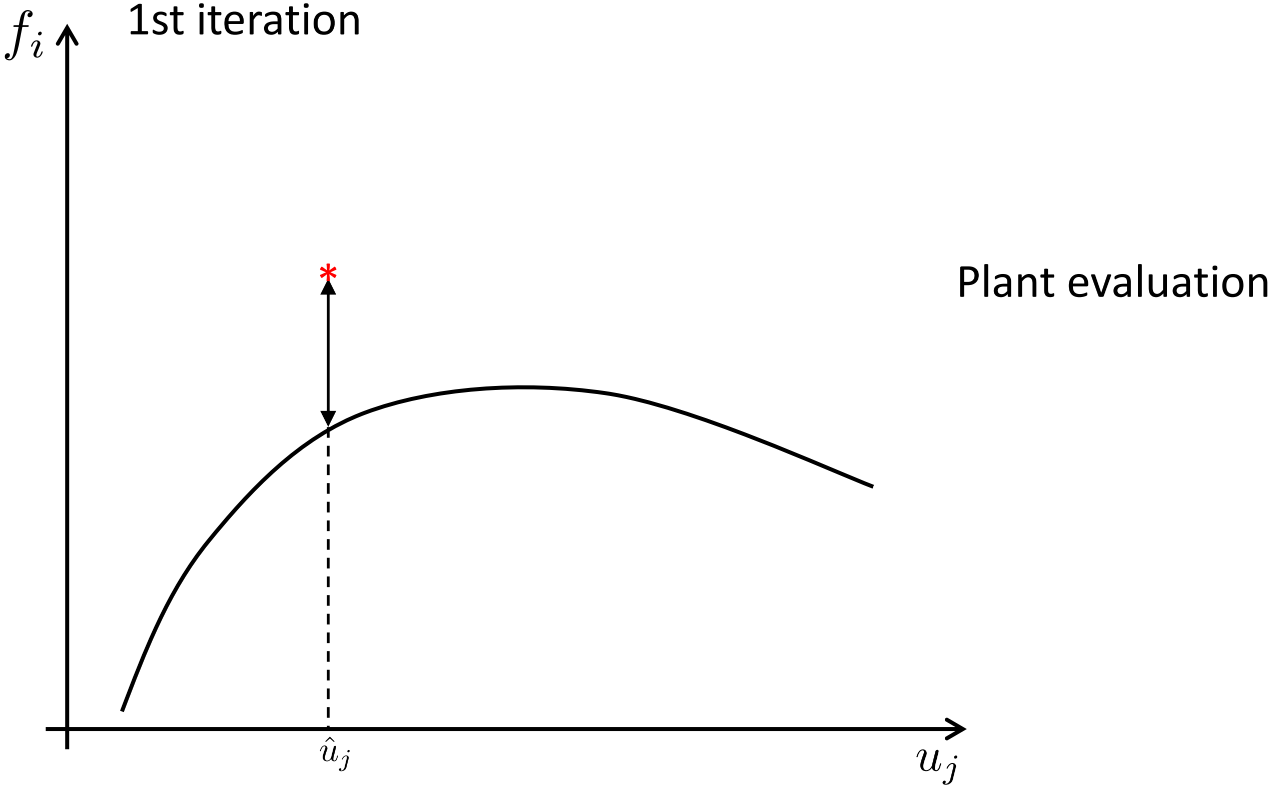

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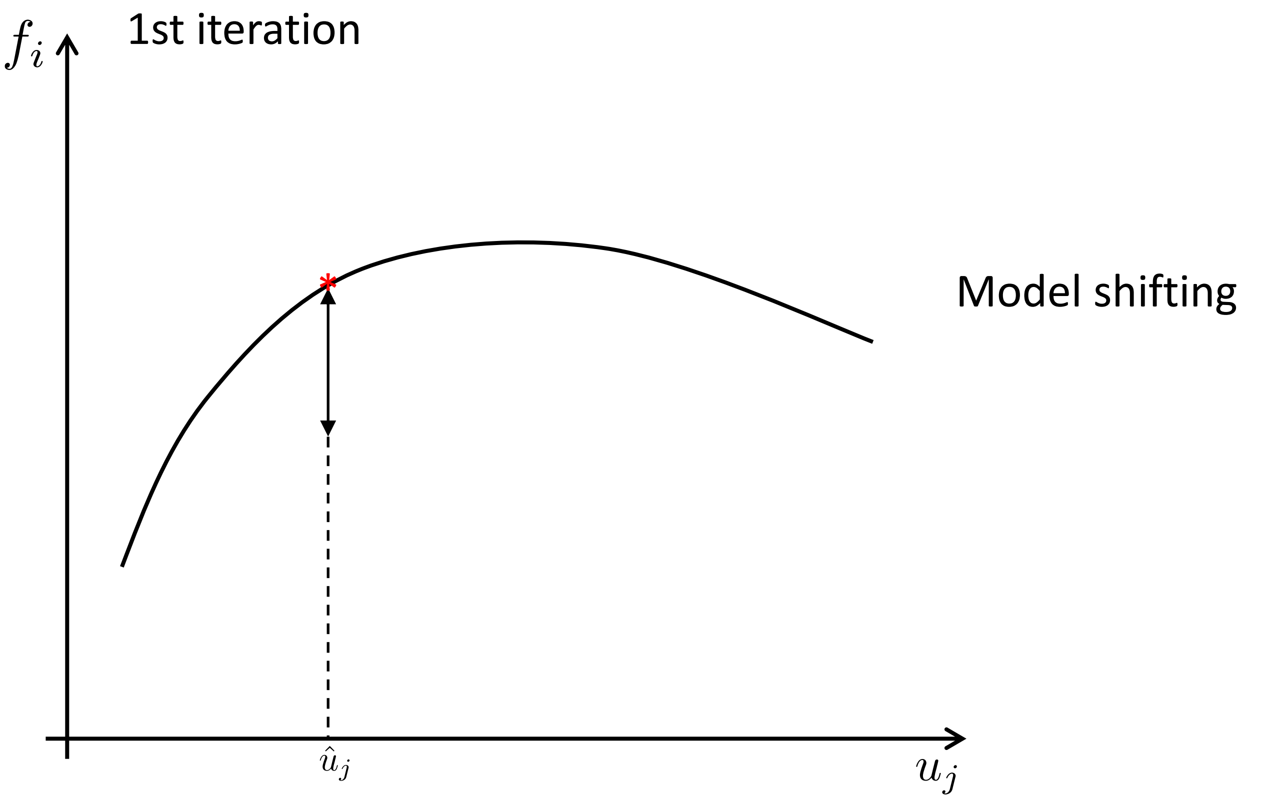

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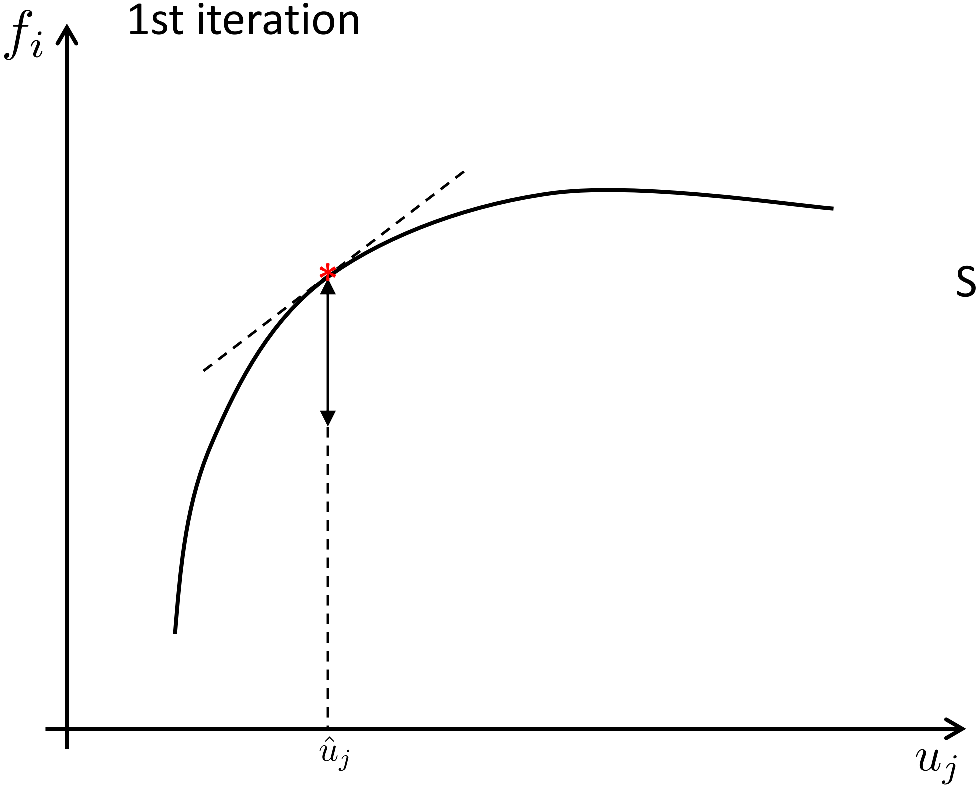
1st iteration



Slop correction

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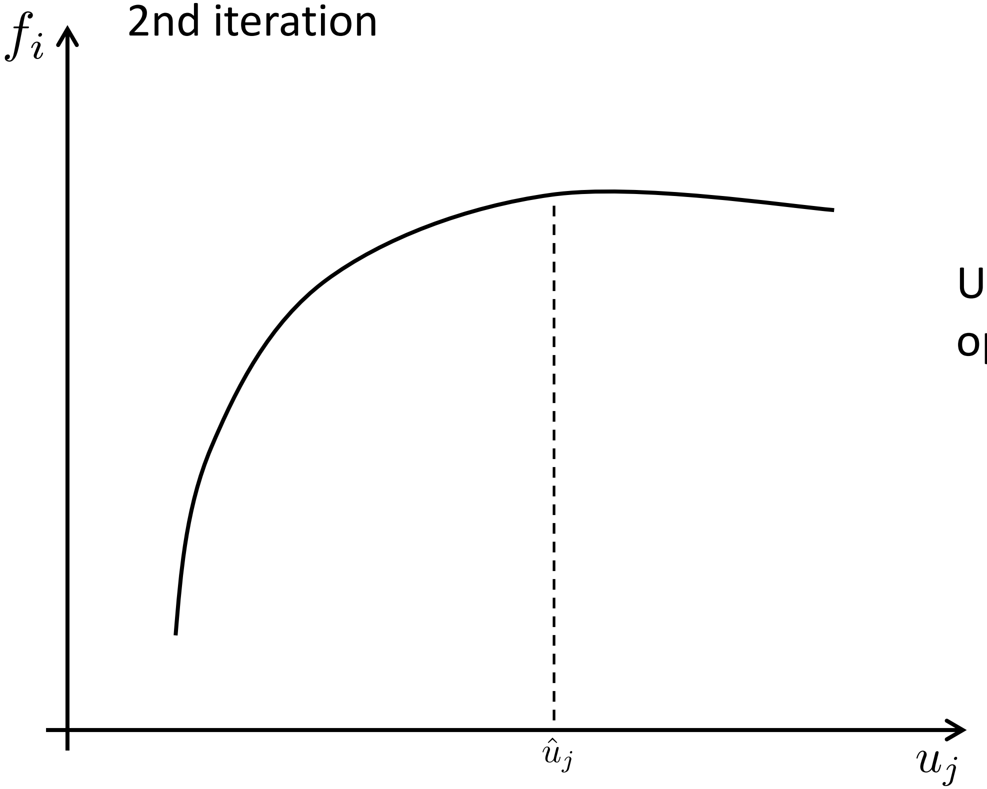

Updated model optimization

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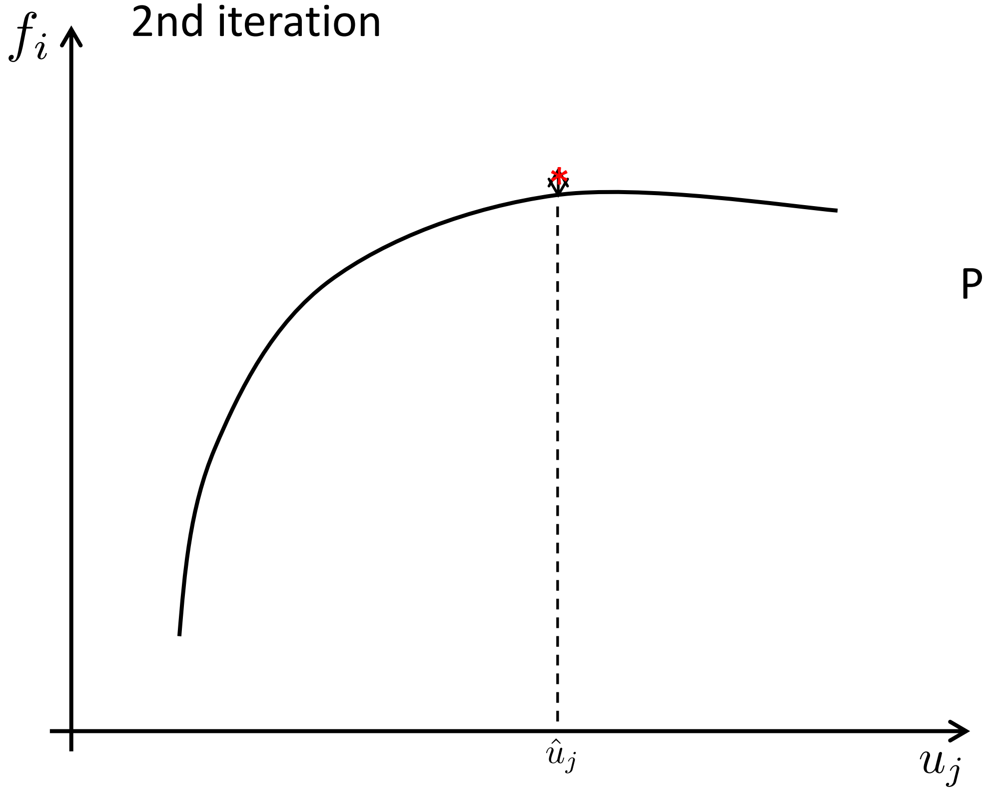

Plant evaluation

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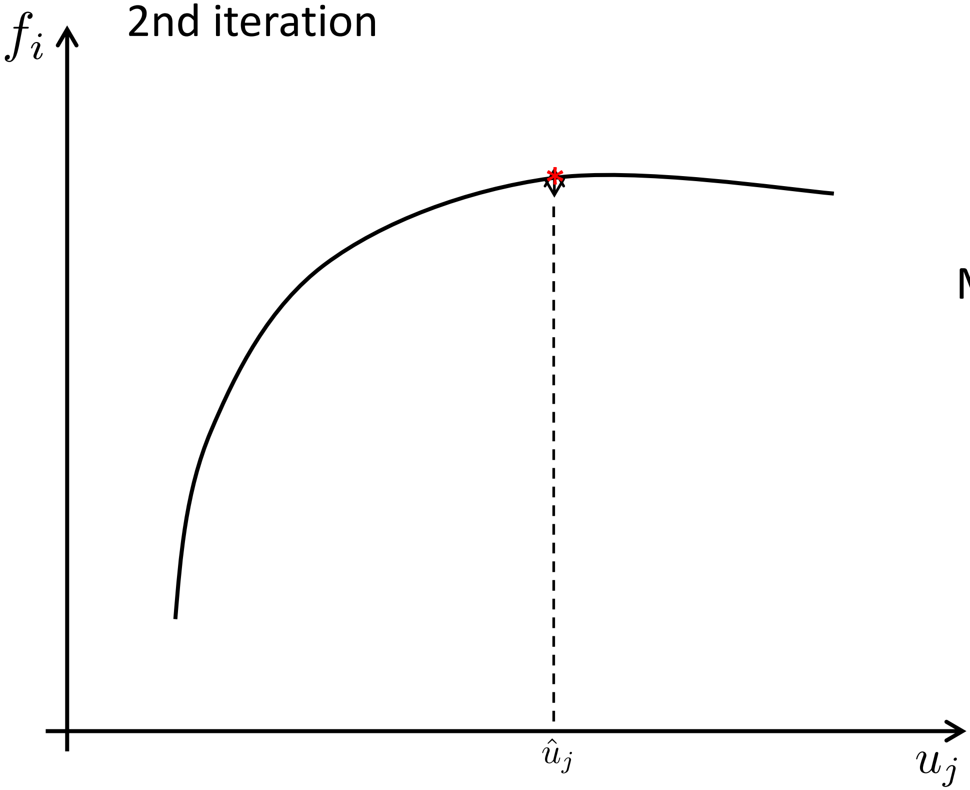

Model shifting

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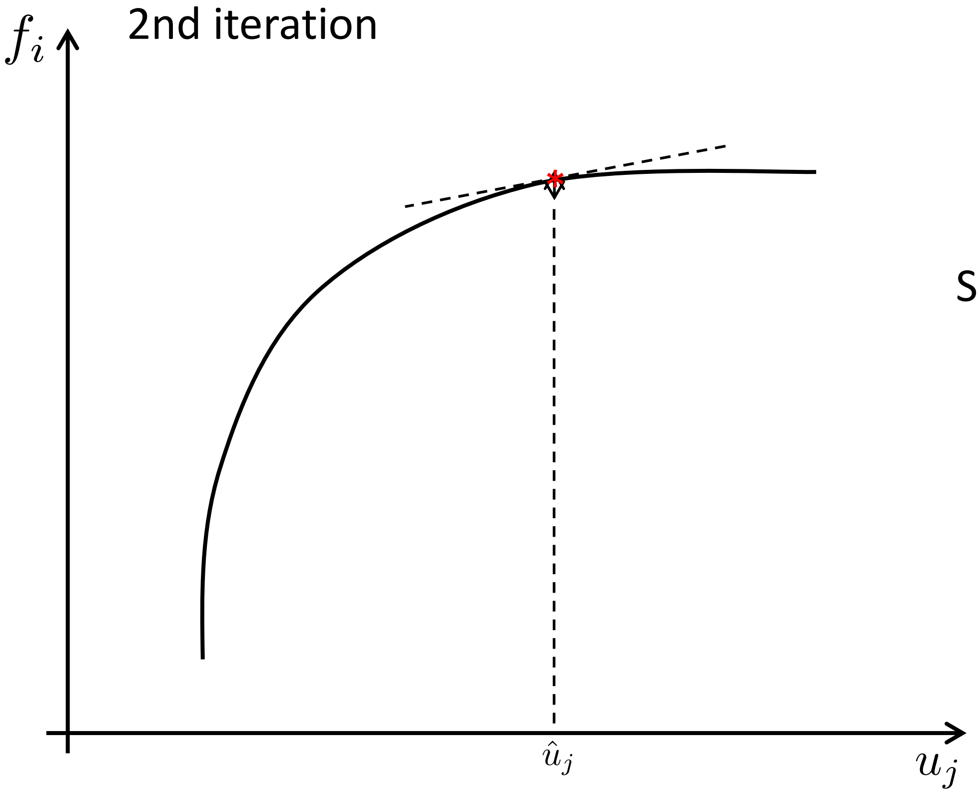

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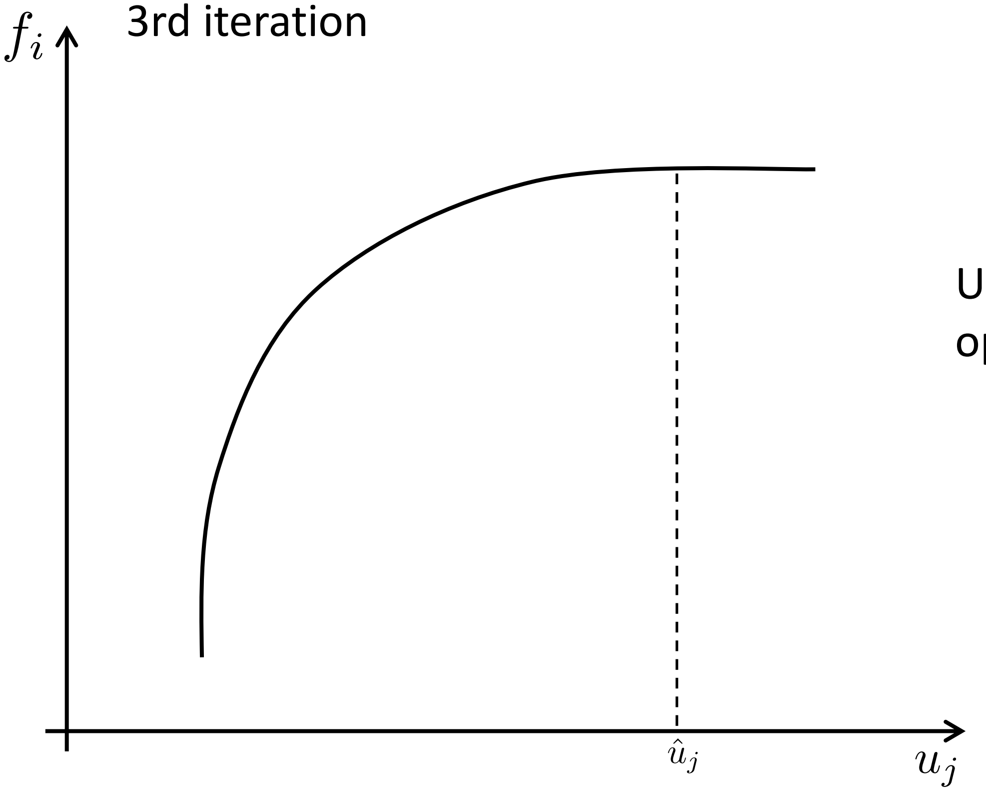

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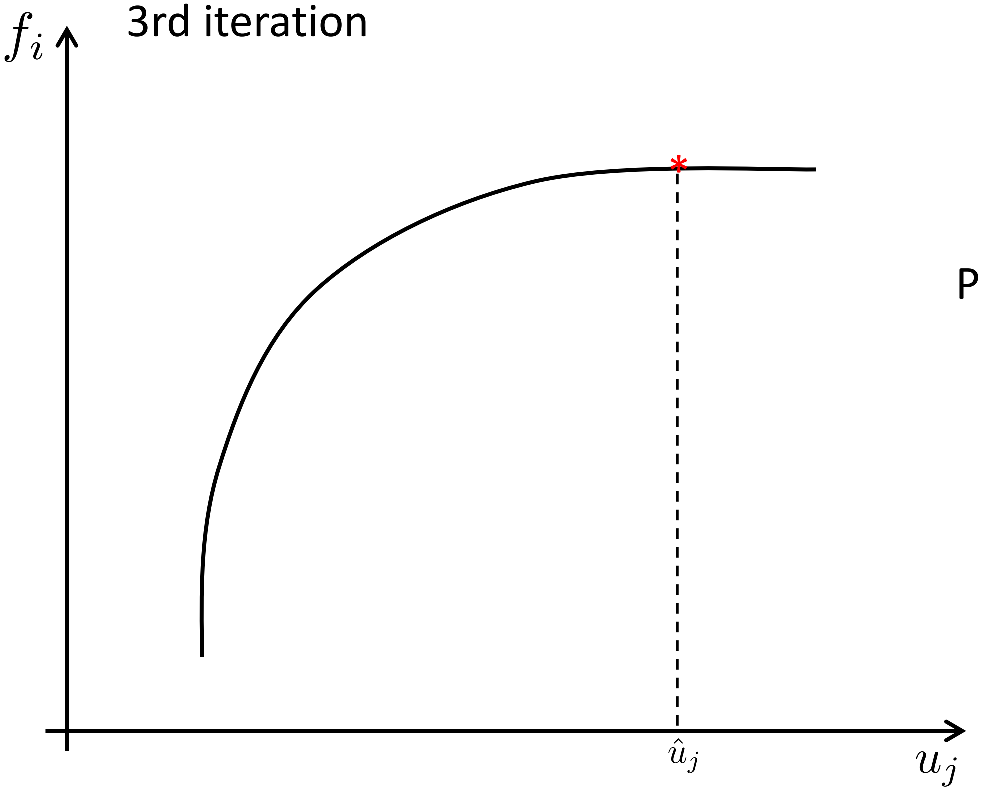

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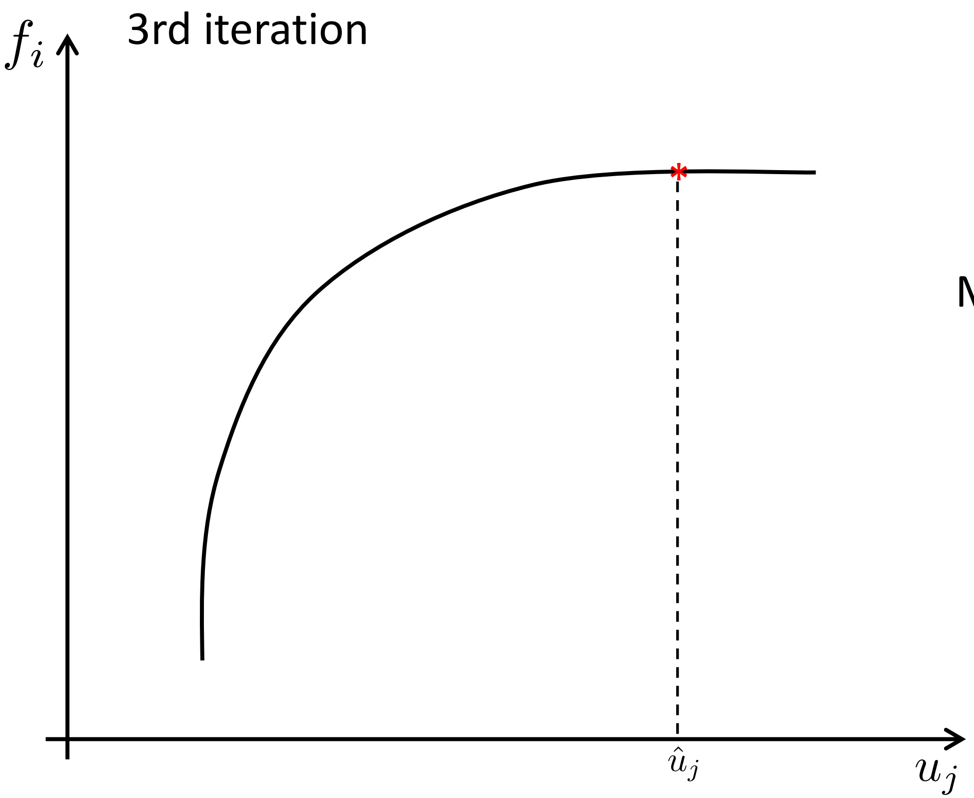

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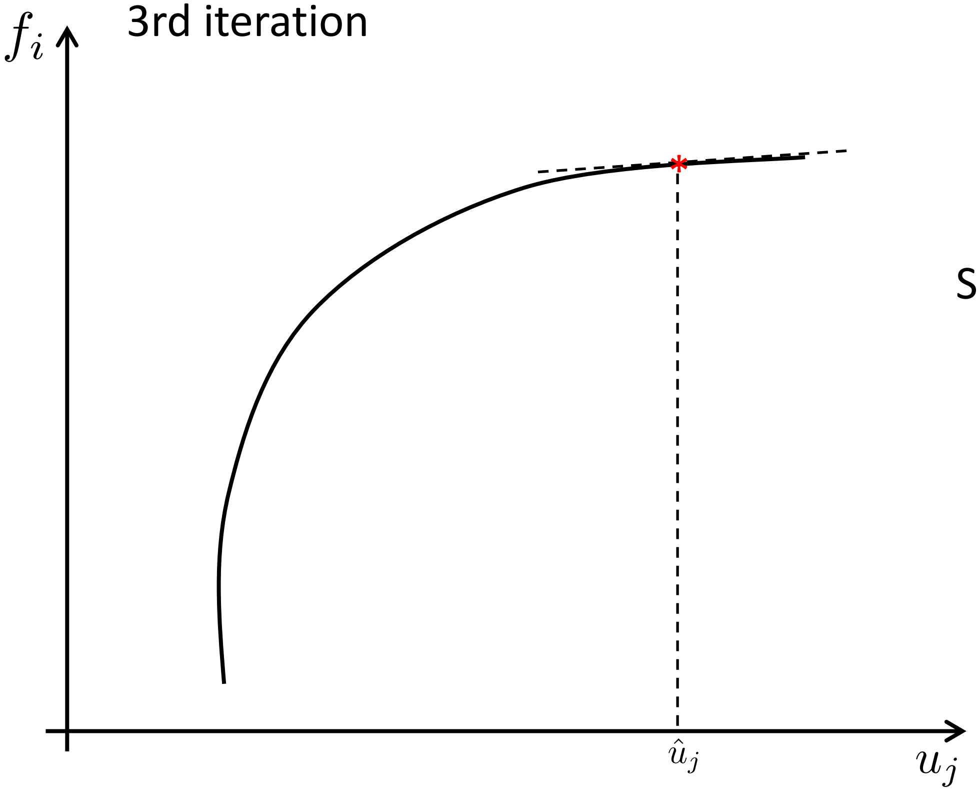

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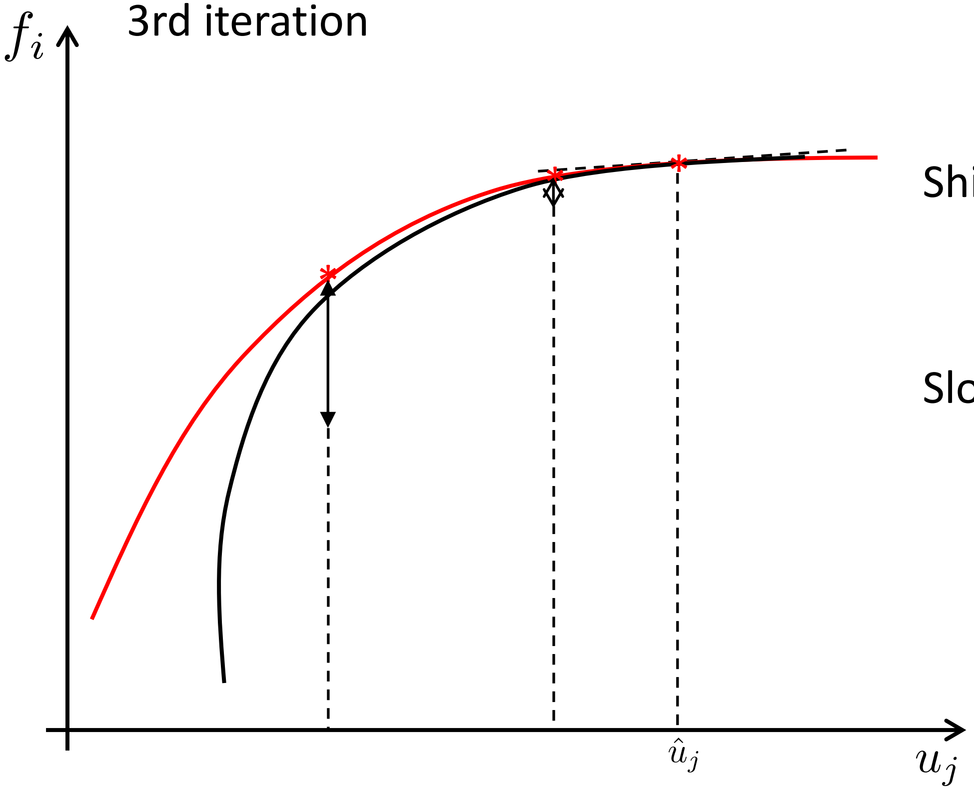

Shifting correction:

$$\varepsilon_k^f = f_p(u_k) - f(u_k)$$

Slope correction:

$$\underbrace{\left(\frac{\partial f_p}{\partial u}(u_k) - \frac{\partial f}{\partial u}(u_k)\right)}_{\lambda^f}(u - u_k)$$

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Modifier-Adaptation Scheme

The modified optimization problem can be written as follows:

$$\mathbf{u}_{k+1}^* \in \arg\min_{\mathbf{u}} \Phi_{m,k}(\mathbf{u})$$
$$\text{s.t} \quad G_{m,i,k}(\mathbf{u}) \leq \mathbf{0} \qquad (1a)$$
$$\mathbf{u}^L \leq \mathbf{u} \leq \mathbf{u}^U$$

Where the modified constraint and cost functions can be written as

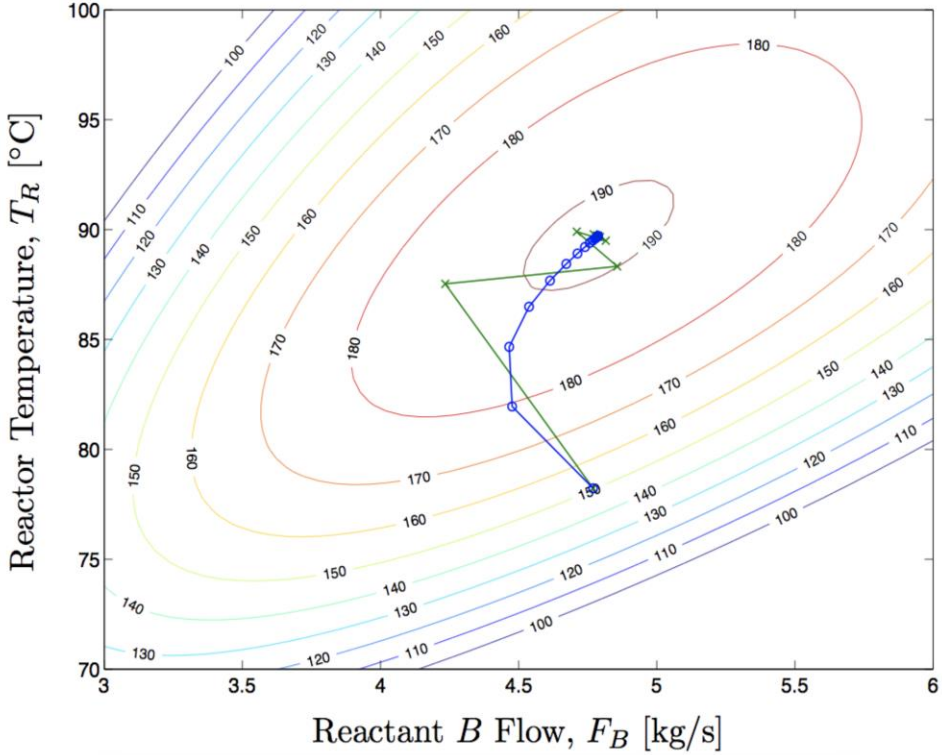
$$\Phi_{m,k}(\mathbf{u}) := \Phi(\mathbf{u}) + \varepsilon_k^{\Phi} + (\boldsymbol{\lambda}_k^{\Phi})^{\mathsf{T}}(\mathbf{u} - \mathbf{u}_k)$$
$$G_{m,i,k}(\mathbf{u}) := G_i(\mathbf{u}) + \varepsilon_k^{G_i} + (\boldsymbol{\lambda}_k^{G_i})^{\mathsf{T}}(\mathbf{u} - \mathbf{u}_k) \leq 0, \quad i = 1, \ldots, n_g, \qquad (1b)$$

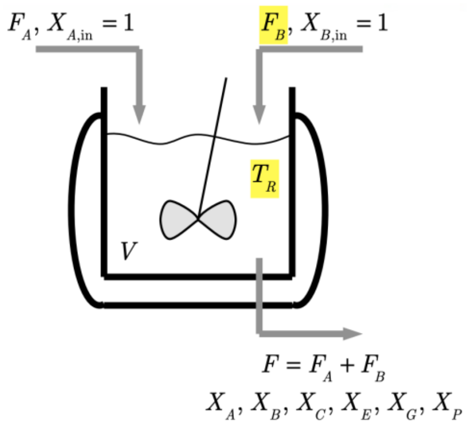
The zeroth- and first-order modifiers are

$$\varepsilon_k^{\Phi} = \Phi_p(\mathbf{u}_k) - \Phi(\mathbf{u}_k),$$
$$\varepsilon_k^{G_i} = G_{p,i}(\mathbf{u}_k) - G_i(\mathbf{u}_k), \quad i = 1, \ldots, n_g,$$
$$(\boldsymbol{\lambda}_k^{\Phi})^{\mathsf{T}} = \frac{\partial \Phi_p}{\partial \mathbf{u}}(\mathbf{u}_k) - \frac{\partial \Phi}{\partial \mathbf{u}}(\mathbf{u}_k), \qquad (1c)$$
$$(\boldsymbol{\lambda}_k^{G_i})^{\mathsf{T}} = \frac{\partial G_{p,i}}{\partial \mathbf{u}}(\mathbf{u}_k) - \frac{\partial G_i}{\partial \mathbf{u}}(\mathbf{u}_k), \quad i = 1, \ldots, n_g.$$

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!

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

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 Problem (1) 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.*

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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.

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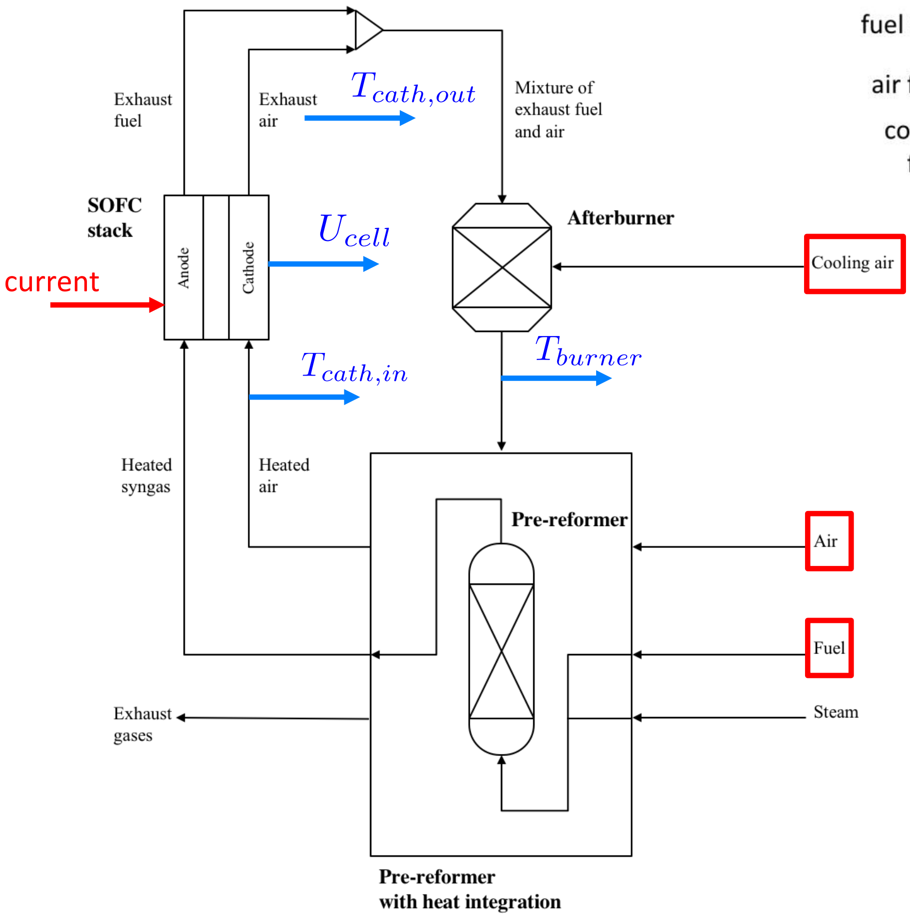
Experimental Real-Time Optimization

RTO of a **Commercial** SOFC System

BlueGEN System



Operational Constraints

Constraint	Lower bound	Upper bound
U_{cell} [V]	0.76	-
ν [-]	-	0.8
λ_{air} [-]	3	-
$T_{cath,in}$ [°C]	650	750
$T_{cath,out}$ [°C]	650	790
T_{burner} [°C]	-	890
q_{CH4} [$L.min^{-1}$]	1	7
q_{air} [$L.min^{-1}$]	85	200
I [A]	0	50
q_{cool} [$L.min^{-1}$]	0	40

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de Avila Ferreira, T., Wuillemin, Z., Faulwasser, T., Salzmann, C. and Bonvin, D., 2019. Enforcing optimal operation in solid-oxide fuel-cell systems. *Energy*, *181*, pp.281-293.

Optimization problem for the SOFC System

$$\max_{\mathbf{u}} \quad \eta_{sys}(\mathbf{u}) = \frac{P_{el}}{q_{CH_4}\ LHV_{CH_4}}$$

$$\text{s.t. steady-state model equations}$$

$$P_{el}(\mathbf{u}) + \underline{\varepsilon^{P_{el}}} = P_{el}^S\ [W]$$

$$U_{cell}(\mathbf{u}) + \underline{\varepsilon^{U_{cell}}} \geq 0.76\ [V]$$

$$650 \leq T_{cath,in}(\mathbf{u}) + \underline{\varepsilon^{T_{cath,in}}} \leq 750\ [°C]$$

$$650 \leq T_{cath,out}(\mathbf{u}) + \underline{\varepsilon^{T_{cath,out}}} \leq 790\ [°C]$$

$$T_{burner}(\mathbf{u}) + \underline{\varepsilon^{T_{burner}}} \leq 890\ [°C]$$

$$\nu(\mathbf{u}) \leq 0.8$$

$$\lambda_{air}(\mathbf{u}) \geq 3$$

$$1 \leq q_{CH_4} \leq 7\ [L.min^{-1}]$$

$$85 \leq q_{air} \leq 200\ [L.min^{-1}]$$

$$0 \leq I \leq 50\ [L.min^{-1}]$$

$$0 \leq q_{cool} \leq 40\ [L.min^{-1}]$$

Electrical Power Profile 1:

$$\tau_{RTO} = 90 \text{ min}$$

$$P_{el}^S(t) = \begin{cases} 1000\ [W], & \text{t} \leq 24 \text{ h} \\ 1250\ [W], & 24 \text{ h} < \text{t} \leq 48 \text{ h} \\ 1500\ [W], & \text{t} > 48 \text{ h.} \end{cases}$$

Electrical Power Profile 2:

$$\tau_{RTO} = 5 \text{ min}$$

$$P_{el}^S(t) = \begin{cases} 1000\ [W], & \text{t} \leq 2 \text{ h} \\ 1250\ [W], & 2 \text{ h} < \text{t} \leq 4 \text{ h} \\ 1500\ [W], & \text{t} > 4 \text{ h.} \end{cases}$$

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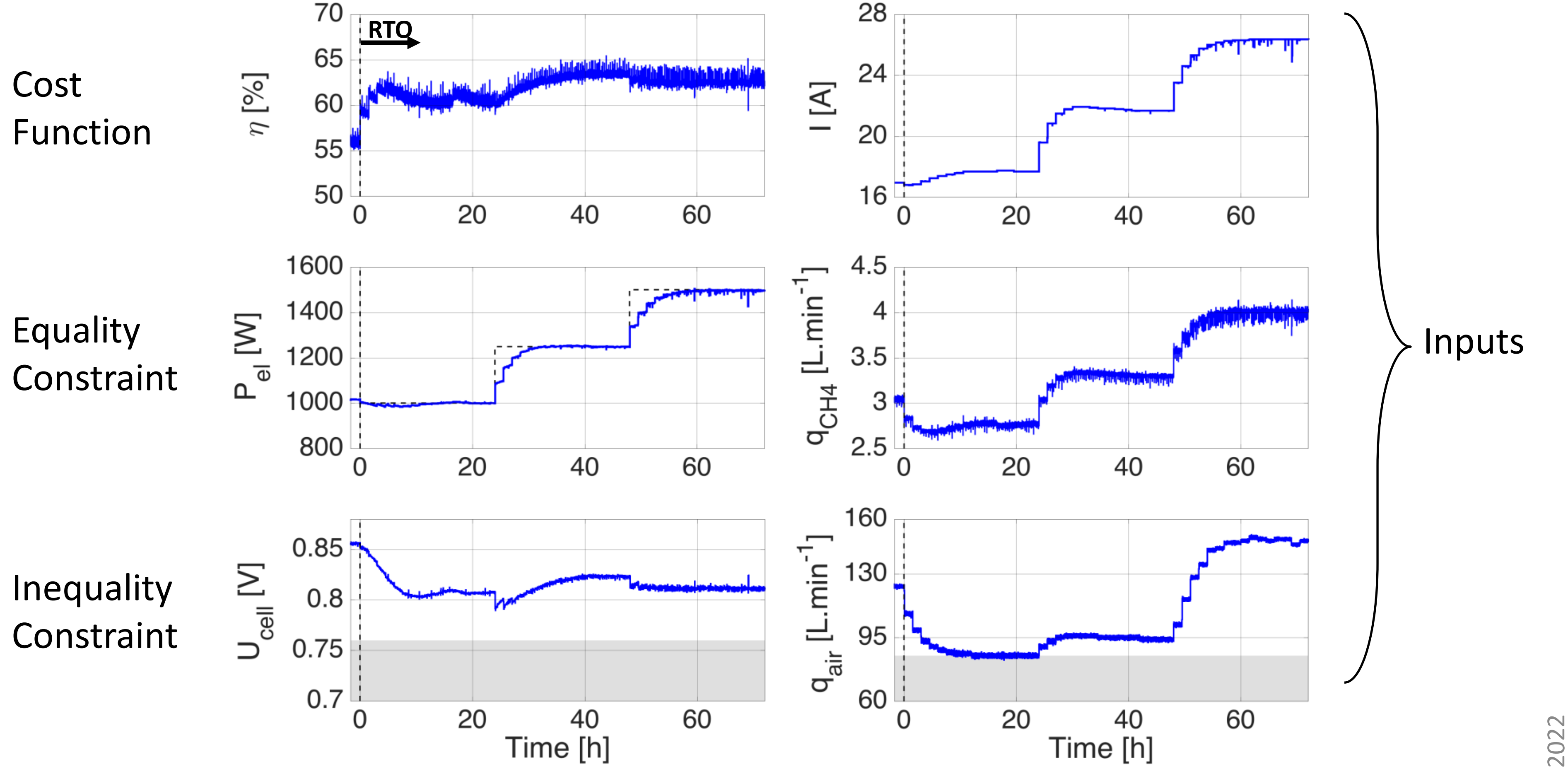
de Avila Ferreira, T., Wuillemin, Z., Faulwasser, T., Salzmann, C. and Bonvin, D., 2019. Enforcing optimal operation in solid-oxide fuel-cell systems. *Energy*, *181*, pp.281-293.

Experimental Results: **Steady-State CA (Profile 1)**

Exp. 1: *CA_ss, τ_{RTO} = 90 min and 72-h Experiment*



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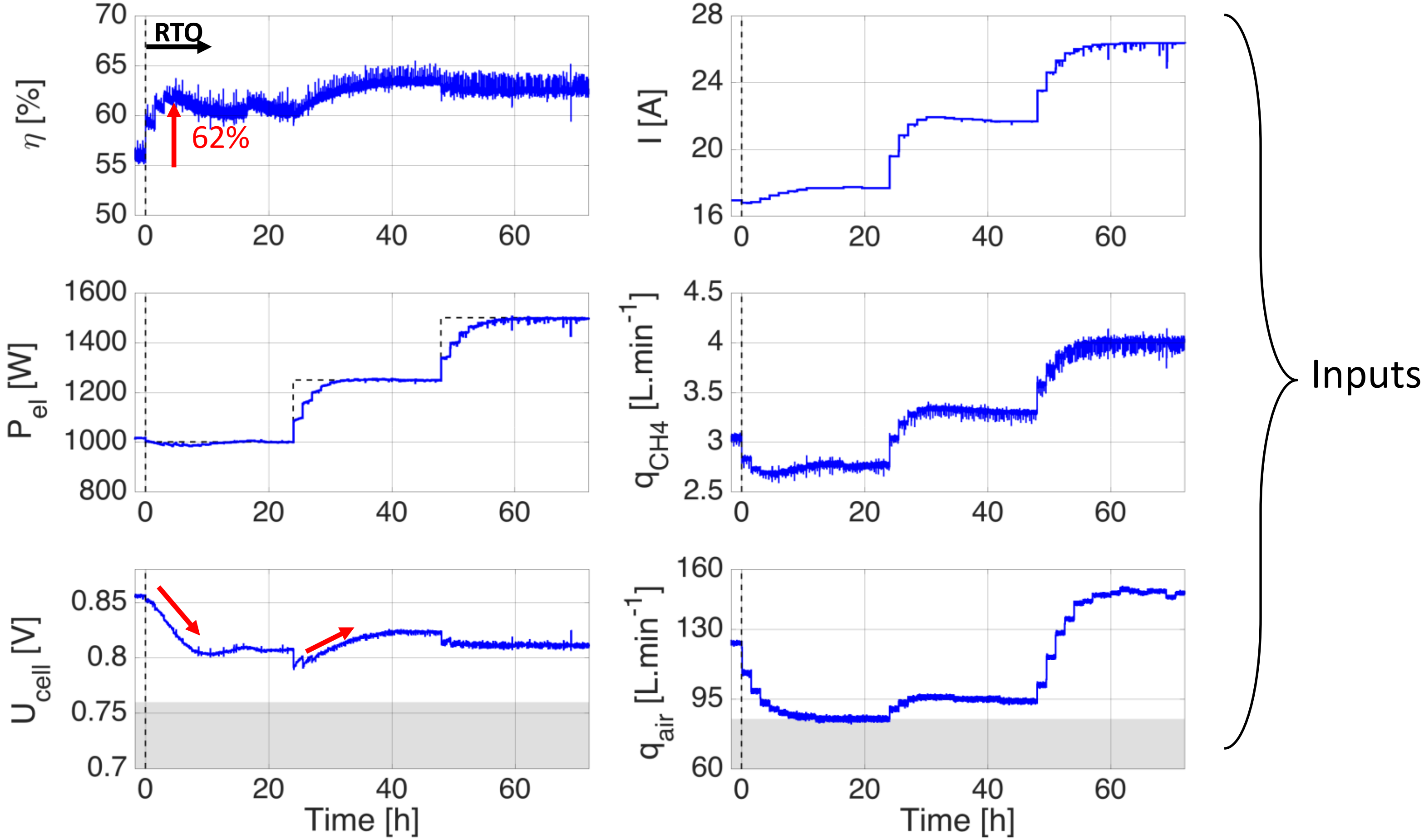
Cost Function

Equality Constraint

Inequality Constraint



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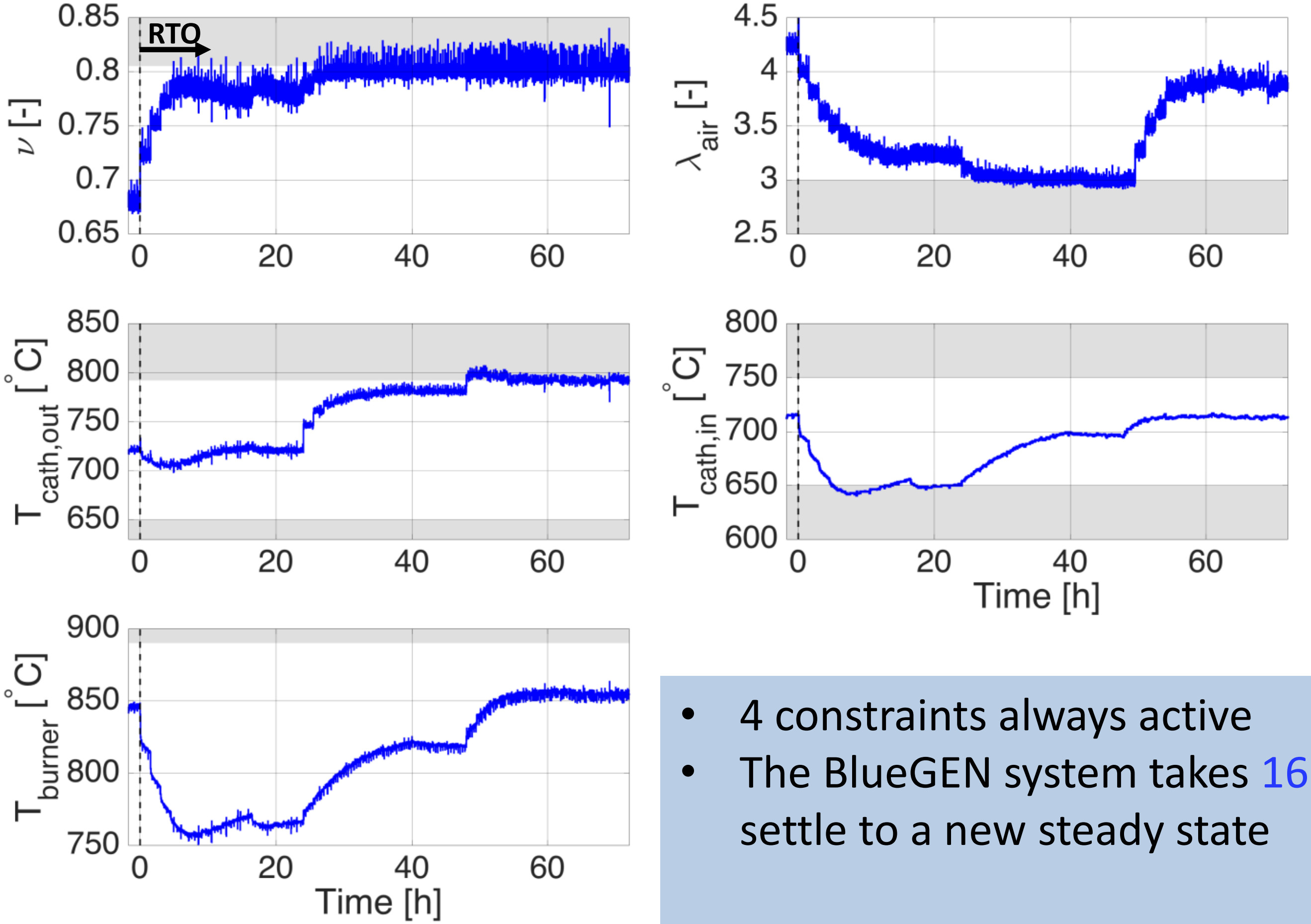

- 4 constraints always active
- The BlueGEN system takes 16 to 20 h to settle to a new steady state

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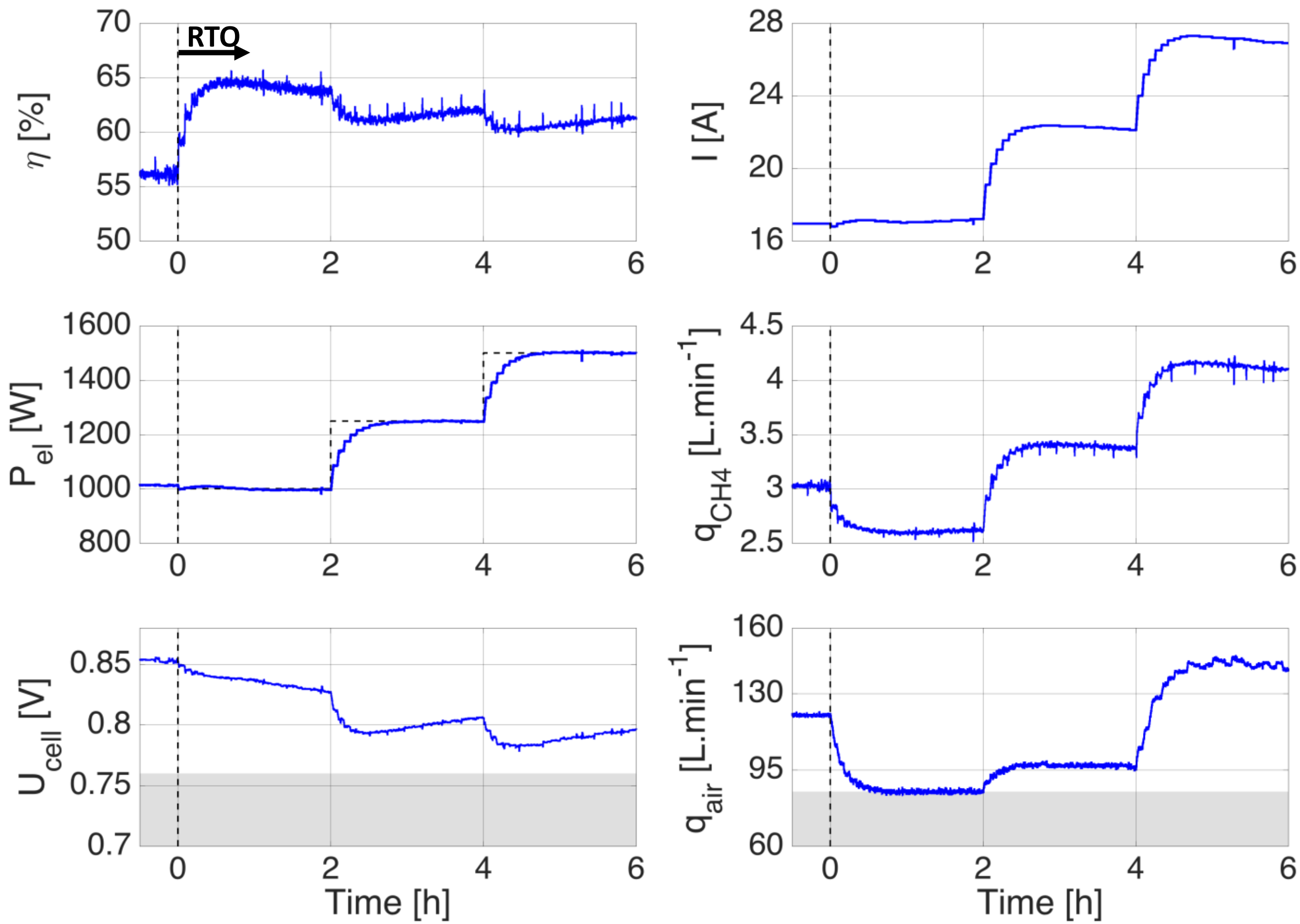
Experimental Results: **Fast CA (Profile 2)**

Exp. 2: *CA_dyn, τ_{RTO} = 5 min and 6-h Experiment*

Cost Function

Equality Constraint

Inequality Constraint



Inputs

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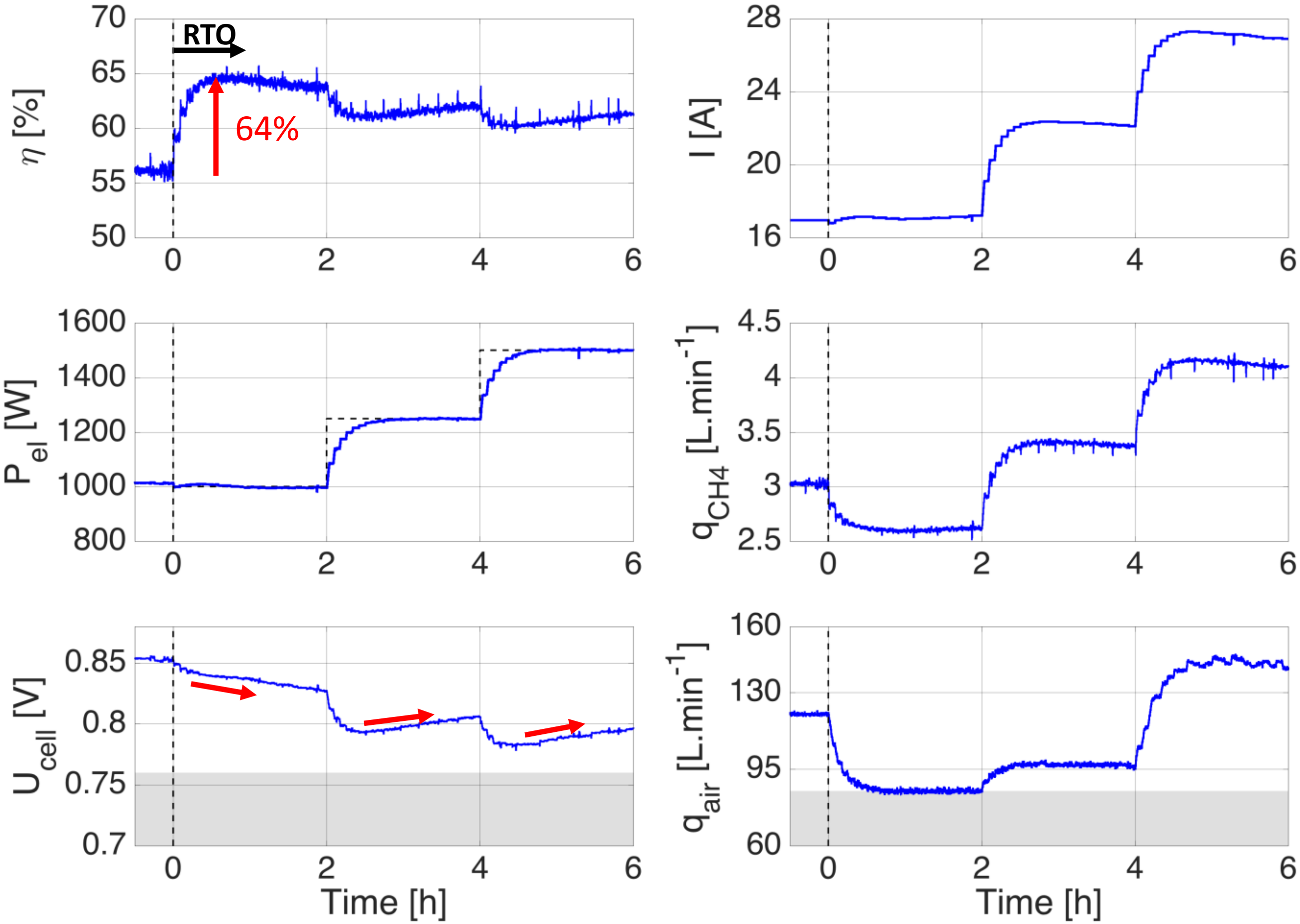

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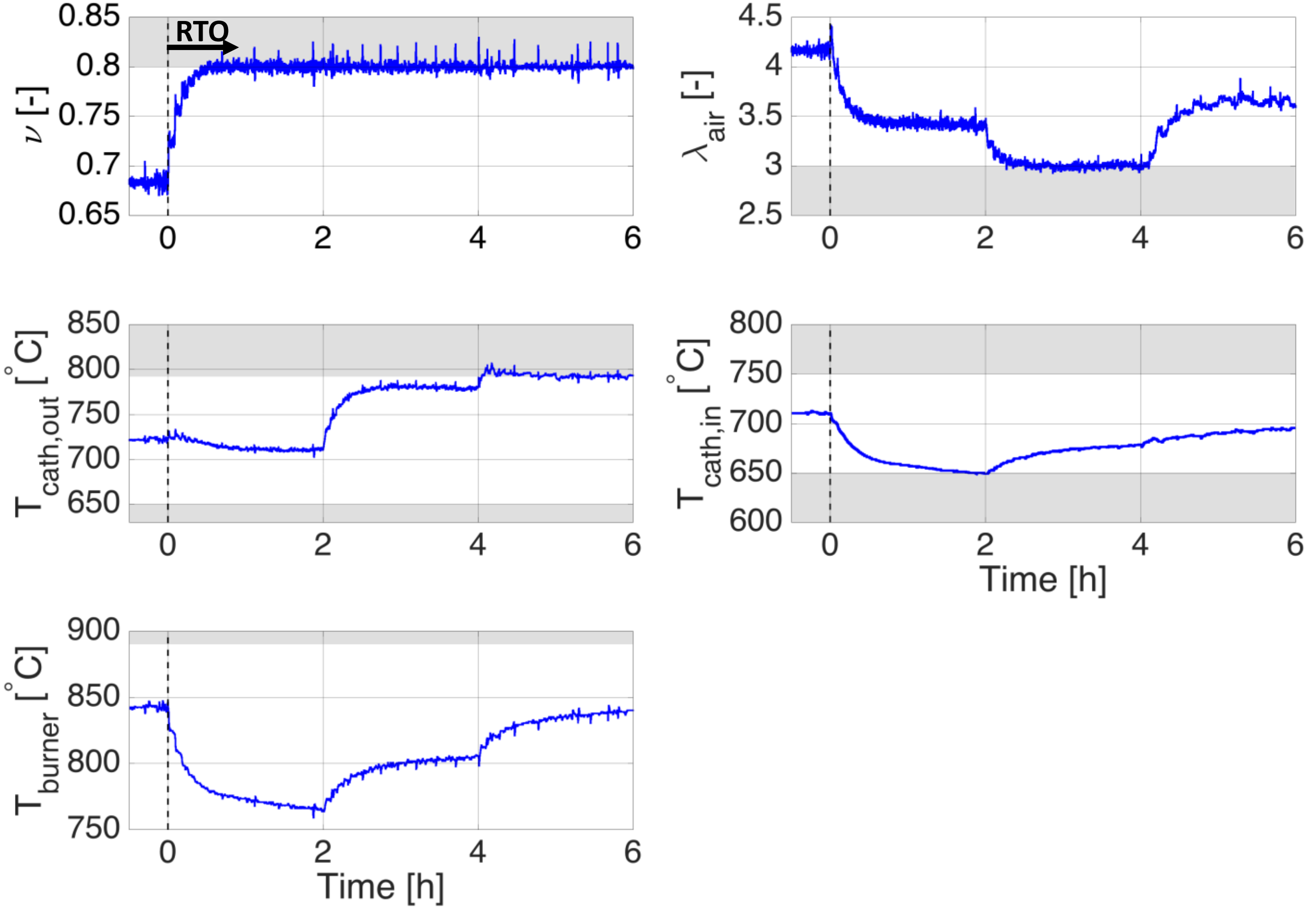

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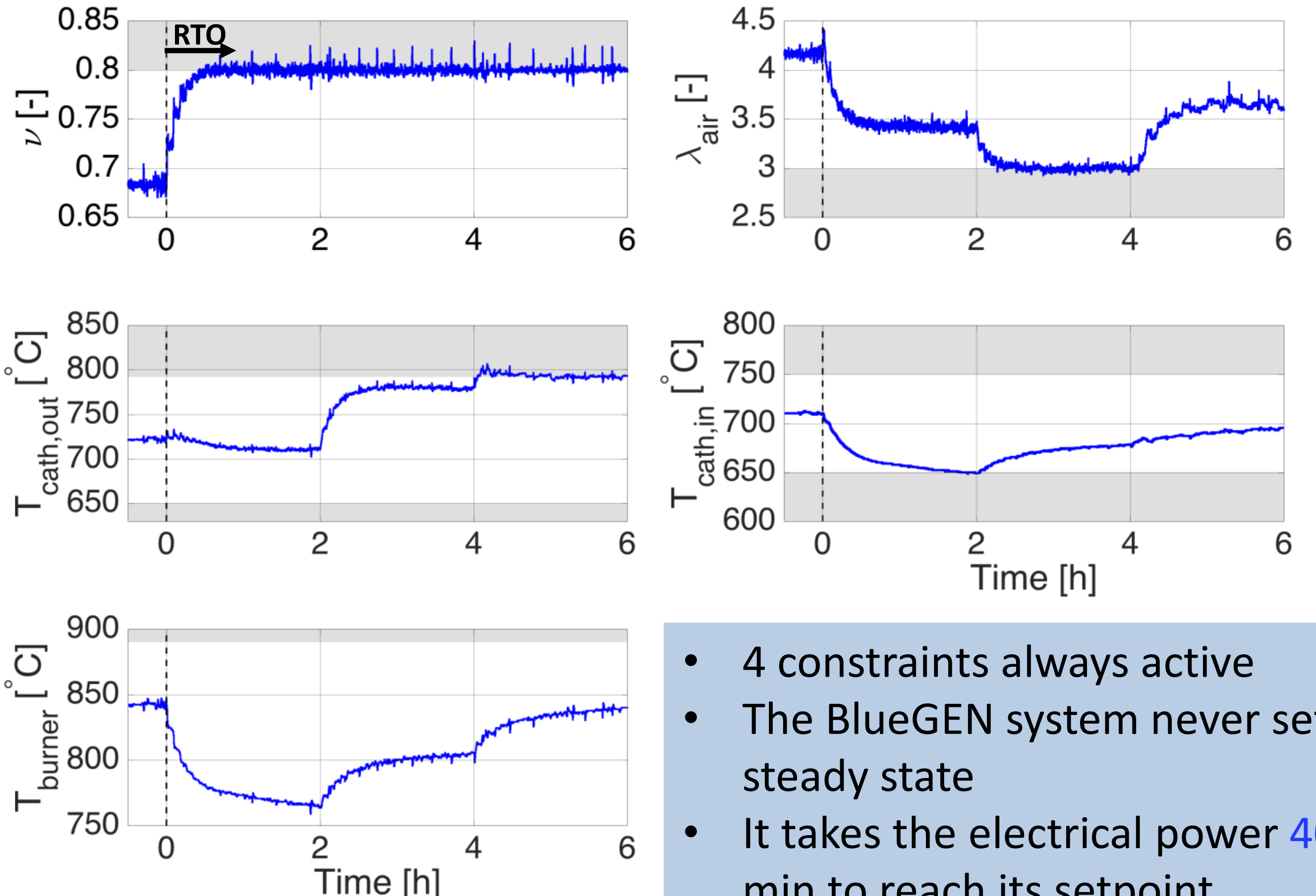

- 4 constraints always active
- The BlueGEN system never settles to a steady state
- It takes the electrical power 40 to 45 min to reach its setpoint

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Conclusions

- RTO is a family of optimization methods that incorporate process measurements in the optimization framework to drive a real process to optimal performance
- We develop 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 fuel cells and degrading 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)
- We will apply RTO in both RUBY (SOFC) and REACTT (SOE)

Thank you!

Funded by the EU Fuel Cell and Hydrogen 2 Joint Undertaking - H2020 Programme Grant Agreement Number 875047.

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