

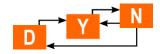


## Experimental Real Time Optimization of a Continuous Membrane Separation Plant

Anwesh Reddy Gottu Mukkula<sup>1</sup>, Petra Valiauga<sup>2</sup>, Miroslav Fikar<sup>2</sup>, Radoslav Paulen<sup>2</sup>, Sebastian Engell<sup>1</sup>

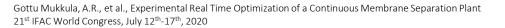
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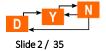




Motivation	Real-time optimization	Modifier adaptation with quadratic approximation (MAWQA)	Case study	Summary	
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Containerized reactor module					

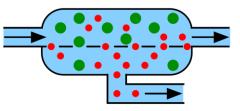






Motivation	Real-time optimization	Modifier adaptation with quadratic approximation (MAWQA)	Case study	Summary	
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Containerized reactor module					

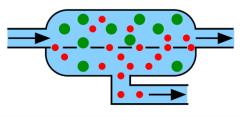






Motivation	Real-time optimization	Modifier adaptation with quadratic approximation (MAWQA)	Case study	Summary
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Containerized reactor module				





#### Goal

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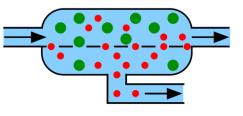
- Identify the optimal operating input for a nanofiltration membrane separation process
- Process and productivity constraints have to be taken into account



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Motivation	Real-time optimization	Modifier adaptation with quadratic approximation (MAWQA)	Case study	Summary	
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Containerized reactor module					





#### Goal

- Identify the optimal operating input for a nanofiltration membrane separation process
- Process and productivity constraints have to be taken into account

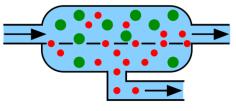
#### Plant:

 $\mathbf{u}_p^* = \min_{\mathbf{u}} \mathcal{J}_p(\mathbf{y}, \mathbf{u})$ s.t.  $\mathbf{y} = \mathbf{f}_p(\mathbf{u})$ 



Motivation	Real-time optimization	Modifier adaptation with quadratic approximation (MAWQA)	Case study	Summary	
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Containerized reactor module					





#### Goal

- Identify the optimal operating input for a nanofiltration membrane separation process
- Process and productivity constraints have to be taken into account

Plant:  

$$\mathbf{u}_p^* = \min_{\mathbf{u}} \mathcal{J}_p(\mathbf{y}, \mathbf{u})$$
  
s.t.  $\mathbf{y} = \mathbf{f}_p(\mathbf{u})$ 

#### Challenge

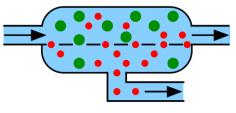
Unknown process model



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Motivation	Real-time optimization	Modifier adaptation with quadratic approximation (MAWQA)	Case study	Summary
•	0	0000	0000	0
Motivation				





#### Goal

- Identify the optimal operating input for a nanofiltration membrane separation process
- Process and productivity constraints have to be taken into account

## Plant: $\mathbf{u}_p^* = \min_{\mathbf{u}} \mathcal{J}_p(\mathbf{y}, \mathbf{u})$ s.t. $\mathbf{y} = \mathbf{f}_p(\mathbf{u})$

#### Challenge

Unknown process model

#### **Proposed solution**

Real-time optimization methods



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Motivation	Real-time optimization	Modifier adaptation with quadratic approximation (MAWQA)	Case study	Summary	
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Real-time optimization methods					

## Real-time optimization

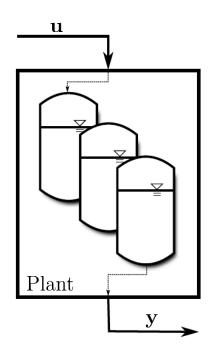
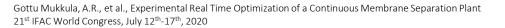


Figure: Illustration of a general plant.

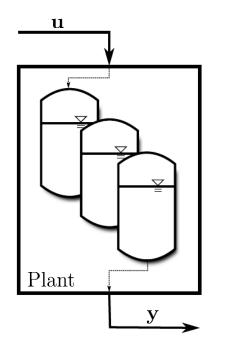




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Motivation	Real-time optimization	Modifier adaptation with quadratic approximation (MAWQA)	Case study	Summary	
0	•	0000	0000	0	
Real-time optimization methods					

### Real-time optimization



$$\mathbf{u}_p^* = \min_{\mathbf{u}} \mathcal{J}_p(\mathbf{y}, \mathbf{u})$$
  
s.t.  $\mathbf{y} = \mathbf{f}_p(\mathbf{u})$ 

Model:

$$\mathbf{u}_m^* = \min_{\mathbf{u}} \mathcal{J}_m(\hat{\mathbf{y}}, \mathbf{u})$$
  
s.t.  $\hat{\mathbf{y}} = \mathbf{f}_m(\mathbf{u})$ 

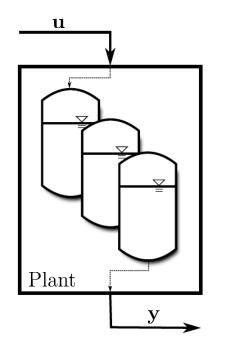
 $\mathbf{u}_m^* \neq \mathbf{u}_p^*$ 

Figure: Illustration of a general plant.

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Motivation	Real-time optimization	Modifier adaptation with quadratic approximation (MAWQA)	Case study	Summary	
0	•	0000	0000	0	
Real-time optimization methods					

#### Real-time optimization





$$\begin{aligned} & \underset{\mathbf{u}}{\overset{*}{}_{p}} = \min_{\mathbf{u}} \mathcal{J}_{p}(\mathbf{y}, \mathbf{u}) \\ & \text{s.t. } \mathbf{y} = \mathbf{f}_{p}(\mathbf{u}) \end{aligned}$$

Model:

$$\mathbf{u}_m^* = \min_{\mathbf{u}} \mathcal{J}_m(\hat{\mathbf{y}}, \mathbf{u})$$
  
s.t.  $\hat{\mathbf{y}} = \mathbf{f}_m(\mathbf{u})$ 

 $\mathbf{u}_m^* 
eq \mathbf{u}_p^*$ 

#### **RTO** method

• Modifier adaptation with quadratic approximation (MAWQA)



Figure: Illustration of a general plant.

Motivation	Real-time optimization	Modifier adaptation with quadratic approximation (MAWQA)	Case study	Summary	
0	•	0000	0000	0	
Real-time optimization methods					

Plant:

Model:

 $\mathbf{u}_p^* = \min_{\mathbf{u}} \mathcal{J}_p(\mathbf{y}, \mathbf{u})$ 

 $\mathbf{u}_m^* = \min_{\mathbf{u}} \mathcal{J}_m(\hat{\mathbf{y}}, \mathbf{u})$ 

 $\mathbf{u}_m^* 
eq \mathbf{u}_p^*$ 

s.t.  $\mathbf{y} = \mathbf{f}_p(\mathbf{u})$ 

s.t.  $\hat{\mathbf{y}} = \mathbf{f}_m(\mathbf{u})$ 

#### Real-time optimization

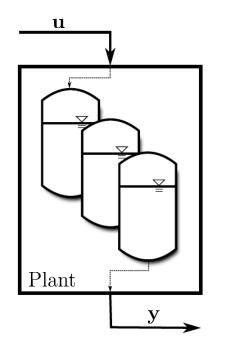
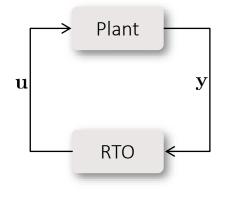


Figure: Illustration of a general plant.

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#### **RTO** method

 Modifier adaptation with quadratic approximation (MAWQA)



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Motivation	Real-time optimization	Modifier adaptation with quadratic approximation (MAWQA)	Case study	Summary
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Modifier adaptation				

### Modifier adaptation (MA)

Model-based optimization

 $\mathbf{u}_{m}^{*} = \min_{\mathbf{u}} \mathcal{J}_{m}(\hat{\mathbf{y}}, \mathbf{u})$ s.t.  $\hat{\mathbf{y}} = \mathbf{f}_{m}(\mathbf{x}, \mathbf{u})$  $\mathbf{g}_{m}(\mathbf{x}, \mathbf{u}) \leq 0$ 

## Modifier adaptation (MA) $\hat{\mathbf{u}}_{m}^{*k+1} = \min_{\mathbf{u}} \mathcal{J}_{m}^{ad,k}(\hat{\mathbf{y}}, \mathbf{u})$ s.t. $\hat{\mathbf{y}} = \mathbf{f}_{m}(\mathbf{x}, \mathbf{u})$ $\mathbf{g}_{m}^{ad,k}(\mathbf{x}, \mathbf{u}) \leq 0$

Motivation	Real-time optimization	Modifier adaptation with quadratic approximation (MAWQA)	Case study	Summary
0	0	000	0000	0
Modifier adaptation				

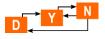
### Modifier adaptation (MA)

Model-based optimization

$$\mathbf{u}_{m}^{*} = \min_{\mathbf{u}} \mathcal{J}_{m}(\hat{\mathbf{y}}, \mathbf{u})$$
  
s.t.  $\hat{\mathbf{y}} = \mathbf{f}_{m}(\mathbf{x}, \mathbf{u})$   
 $\mathbf{g}_{m}(\mathbf{x}, \mathbf{u}) \leq 0$ 

Modifier adaptation (MA)  $\hat{\mathbf{u}}_{m}^{*k+1} = \min_{\mathbf{u}} \mathcal{J}_{m}^{ad,k}(\hat{\mathbf{y}}, \mathbf{u})$ s.t.  $\hat{\mathbf{y}} = \mathbf{f}_{m}(\mathbf{x}, \mathbf{u})$   $\mathbf{g}_{m}^{ad,k}(\mathbf{x}, \mathbf{u}) \leq 0$  Modified objective function and constraints:

$$\begin{aligned} \mathcal{J}_m^{ad,k}(\mathbf{x},\mathbf{u}) &= \mathcal{J}_m(\hat{\mathbf{y}},\mathbf{u}) + (\nabla \mathcal{J}_p^k - \nabla \mathcal{J}_m^k)^T (\mathbf{u} - \mathbf{u}^k) \\ \mathbf{g}_m^{ad,k}(\mathbf{x},\mathbf{u}) &= \mathbf{g}_m(\mathbf{x},\mathbf{u}) + (\mathbf{g}_p^k - \mathbf{g}_m^k) + (\nabla \mathbf{g}_p^k - \nabla \mathbf{g}_m^k)^T (\mathbf{u} - \mathbf{u}^k) \end{aligned}$$



Motivation	Real-time optimization	Modifier adaptation with quadratic approximation (MAWQA)	Case study	Summary
0	0	000	0000	0
Modifier adaptation				

## Modifier adaptation (MA)

Model-based optimization

$$\mathbf{u}_m^* = \min_{\mathbf{u}} \mathcal{J}_m(\hat{\mathbf{y}}, \mathbf{u})$$
  
s.t.  $\hat{\mathbf{y}} = \mathbf{f}_m(\mathbf{x}, \mathbf{u})$   
 $\mathbf{g}_m(\mathbf{x}, \mathbf{u}) \le 0$ 

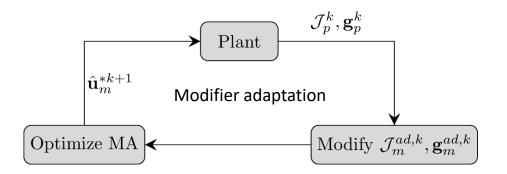
Modifier adaptation (MA)

 $\hat{\mathbf{u}}_m^{*k+1} = \min_{\mathbf{u}} \mathcal{J}_m^{ad,k}(\hat{\mathbf{y}},\mathbf{u})$ 

s.t.  $\hat{\mathbf{y}} = \mathbf{f}_m(\mathbf{x}, \mathbf{u})$ 

Modified objective function and constraints:

$$\mathcal{J}_m^{ad,k}(\mathbf{x}, \mathbf{u}) = \mathcal{J}_m(\hat{\mathbf{y}}, \mathbf{u}) + (\nabla \mathcal{J}_p^k - \nabla \mathcal{J}_m^k)^T (\mathbf{u} - \mathbf{u}^k)$$
$$\mathbf{g}_m^{ad,k}(\mathbf{x}, \mathbf{u}) = \mathbf{g}_m(\mathbf{x}, \mathbf{u}) + (\mathbf{g}_p^k - \mathbf{g}_m^k) + (\nabla \mathbf{g}_p^k - \nabla \mathbf{g}_m^k)^T (\mathbf{u} - \mathbf{u}^k)$$





 $\mathbf{g}_m^{ad,k}(\mathbf{x},\mathbf{u}) \le 0$ 

Motivation	Real-time optimization	Modifier adaptation with quadratic approximation (MAWQA)	Case study	Summary
0	0	000	0000	0
Gradient estimation				

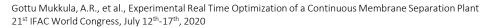
Quadratic approximation (QA)

$$\mathcal{Q}(\mathcal{P}, \mathbf{u}) = \sum_{i=1}^{n_u} \sum_{j=1}^i a_{i,j} u_i u_j + \sum_{i=1}^{n_u} b_i u_i + c$$
$$\mathcal{P} = \{a_{1,1}, \cdots, a_{n_u, n_u}, b_1, \cdots, b_{n_u}, c\}$$

#### Finite differences

- Used for gradient approximation when not enough points are available for fitting a quadratic function
- When number of available points are less than  $\frac{(n_u+1)(n_u+2)}{2}$

[1] Gao, W., Wenzel, S., and Engell, S. (2016), "A reliable modifier-adaptation strategy for real-time optimization", Computers & Chemical Engineering, 91, 318 - 328.





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Motivation	Real-time optimization	Modifier adaptation with quadratic approximation (MAWQA)	Case study	Summary
0	0	0 • 0 0	0000	0
Screening algorithm				

Quadratic approximation (QA)

$$\mathcal{Q}(\mathcal{P}, \mathbf{u}) = \sum_{i=1}^{n_u} \sum_{j=1}^{i} a_{i,j} u_i u_j + \sum_{i=1}^{n_u} b_i u_i + c$$
$$\mathcal{P} = \{a_{1,1}, \cdots, a_{n-n-1}, b_1, \cdots, b_{n-1}c\}$$

 Screening algorithm to choose points for QA

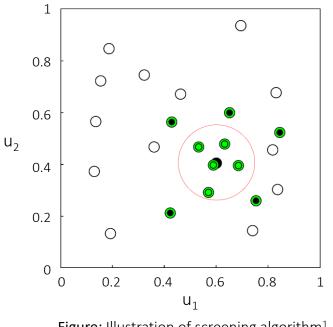


Figure: Illustration of screening algorithm<sup>1</sup>.

Motivation	Real-time optimization	Modifier adaptation with quadratic approximation (MAWQA)	Case study	Summary
0	0	0000	0000	0
Criticality check				

Quadratic approximation (QA)

$$\mathcal{Q}(\mathcal{P}, \mathbf{u}) = \sum_{i=1}^{n_u} \sum_{j=1}^{i} a_{i,j} u_i u_j + \sum_{i=1}^{n_u} b_i u_i + c$$
$$\mathcal{P} = \{a_{1,1}, \cdots, a_{n-n-1}, b_1, \cdots, b_{n-1}, c\}$$

 Screening algorithm to choose points for QA → Criticality Check

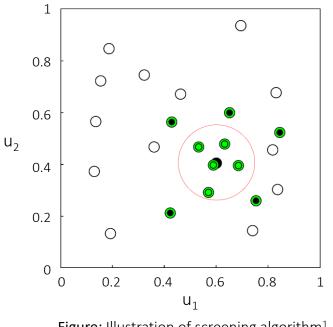


Figure: Illustration of screening algorithm<sup>1</sup>.

Motivation	Real-time optimization	Modifier adaptation with quadratic approximation (MAWQA)	Case study	Summary
0	0	0 • 0 0	0000	0
Trust region constraint				

Quadratic approximation (QA)

$$Q(\mathcal{P}, \mathbf{u}) = \sum_{i=1}^{n_u} \sum_{j=1}^{i} a_{i,j} u_i u_j + \sum_{i=1}^{n_u} b_i u_i + c$$
$$\mathcal{P} = \{a_{1,1}, \cdots, a_{n_u, n_u}, b_1, \cdots, b_{n_u}, c\}$$

- Screening algorithm to choose points for QA
- Additional trust-region constraint:  $(\mathbf{u} - \mathbf{u}^k)^T cov(\mathcal{U}^k)(\mathbf{u} - \mathbf{u}^k) - \gamma^2 \leq 0$

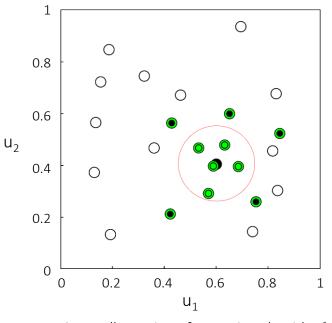


Figure: Illustration of screening algorithm<sup>1</sup>.

Motivation	Real-time optimization	Modifier adaptation with quadratic approximation (MAWQA)	Case study	Summary
0	0	0000	0000	0
Criticality check				

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- Additional trust-region constraint:  $(\mathbf{u} - \mathbf{u}^k)^T cov(\mathcal{U}^k)(\mathbf{u} - \mathbf{u}^k) - \gamma^2 < 0$

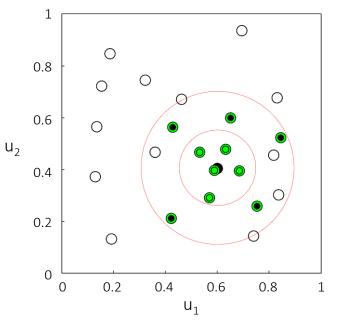


Figure: Illustration of criticality check algorithm<sup>1</sup>.

Motivation	Real-time optimization	Modifier adaptation with quadratic approximation (MAWQA)	Case study	Summary
0	0	0000	0000	0
Criticality check				

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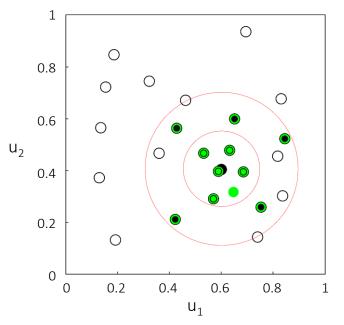


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0	0	0000	0000	0
Criticality check				

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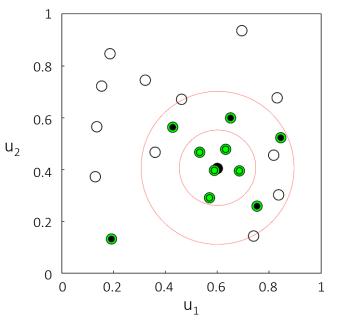


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Motivation	Real-time optimization	Modifier adaptation with quadratic approximation (MAWQA)	Case study	Summary
0	0	0000	0000	0
Criticality check				

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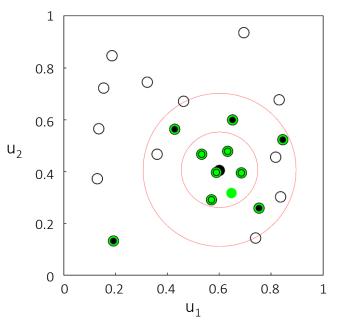


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0	0	0000	0000	0
Criticality check				

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- Additional trust-region constraint:  $(\mathbf{u} - \mathbf{u}^k)^T cov(\mathcal{U}^k)(\mathbf{u} - \mathbf{u}^k) - \gamma^2 < 0$

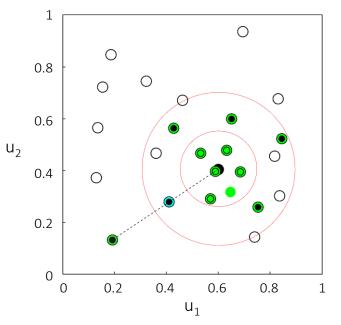


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Motivation	Real-time optimization	Modifier adaptation with quadratic approximation (MAWQA)	Case study	Summary
0	0	000•	0000	0
Criticality check				

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- Screening algorithm to choose points for QA → Criticality Check
- Additional trust-region constraint:  $(\mathbf{u} - \mathbf{u}^k)^T cov(\mathcal{U}^k)(\mathbf{u} - \mathbf{u}^k) - \gamma^2 < 0$

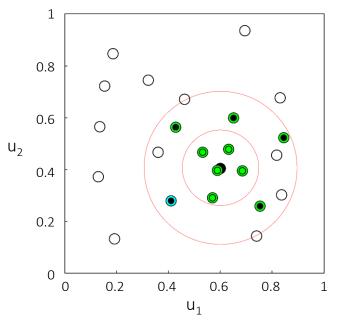
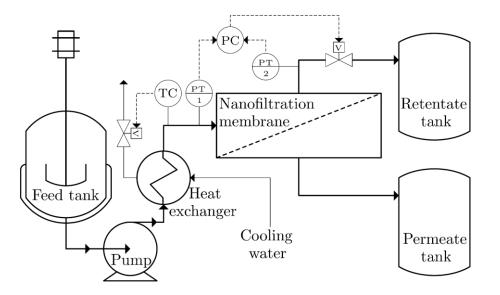


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Motivation	Real-time optimization	Modifier adaptation with quadratic approximation (MAWQA)	Case study	Summary
0	0	0000	• • • •	0
Case study				

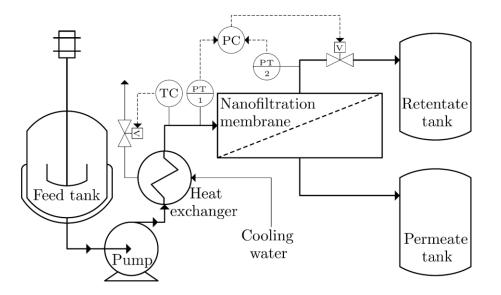
#### Membrane separation process



**Figure:** Illustration of the process flow diagram of the continuously operated membrane separation process.

Motivation	Real-time optimization	Modifier adaptation with quadratic approximation (MAWQA)	Case study	Summary
0	0	0000	• • • •	0
Case study				

#### Membrane separation process



**Figure:** Illustration of the process flow diagram of the continuously operated membrane separation process.

Gottu Mukkula, A.R., et al., Experimental Real Time Optimization of a Continuous Membrane Separation Plant 21<sup>st</sup> IFAC World Congress, July 12<sup>th</sup>-17<sup>th</sup>, 2020

$$\max_{\boldsymbol{u}=\{\Delta P,T\}} \quad \dot{V}_p \kappa_p - 50\Delta P^2 - 5\Delta P(T_{\rm amb} - T)$$

s.t. nominal model,

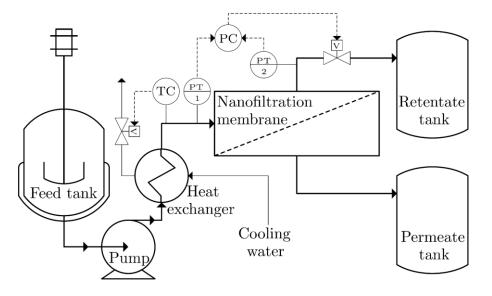
 $18 - \dot{V}_p \le 0,$   $4 \le \Delta P \le 22,$  $20 \le T \le 30.$ 



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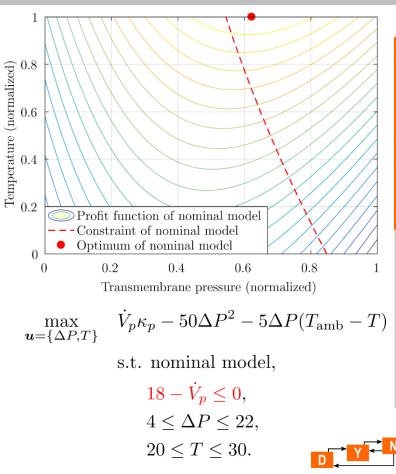
Motivation	Real-time optimization	Modifier adaptation with quadratic approximation (MAWQA)	Case study	Summary
0	0	0000	• • • • •	0
Case study				

#### Membrane separation process



**Figure:** Illustration of the process flow diagram of the continuously operated membrane separation process.

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Motivation	Real-time optimization	Modifier adaptation with quadratic approximation (MAWQA)	Case study	Summary
0	0	0000	$\circ \bullet \circ \circ$	0
Experiment result: Uncons	trained case			

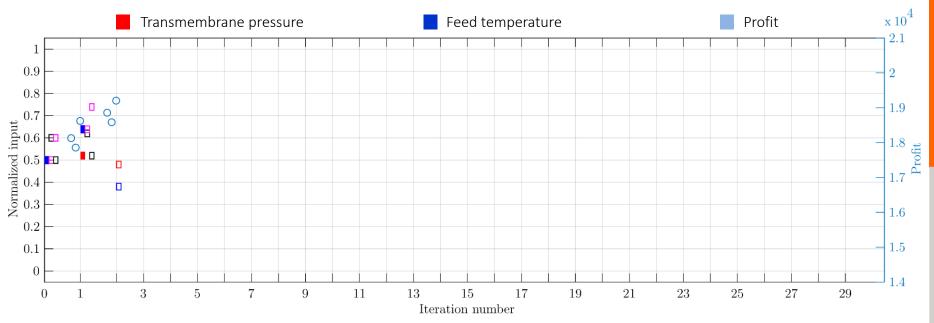


Figure: Experimental results for the unconstrained case: Evolution of the inputs (normalized) transmembrane pressure, temperature and the profit function obtained using process measurements. The tuning parameters  $\gamma$ ,  $\Delta u$ ,  $\Delta h$  and  $\delta$  were set to 3.0, 0.1, 0.1 and 0.1, respectively.



Motivation	Real-time optimization	Modifier adaptation with quadratic approximation (MAWQA)	Case study	Summary
0	0	0000	$\circ \bullet \circ \circ$	0
Experiment result: Uncons	trained case			

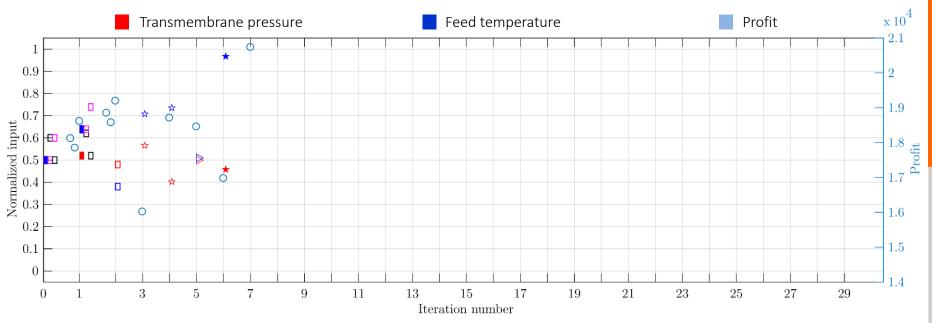


Figure: Experimental results for the unconstrained case: Evolution of the inputs (normalized) transmembrane pressure, temperature and the profit function obtained using process measurements. The tuning parameters  $\gamma$ ,  $\Delta u$ ,  $\Delta h$  and  $\delta$  were set to 3.0, 0.1, 0.1 and 0.1, respectively.

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Motivation	Real-time optimization	Modifier adaptation with quadratic approximation (MAWQA)	Case study	Summary
0	0	0000	$\circ \bullet \circ \circ$	0
Experiment result: Unconst	rained case			

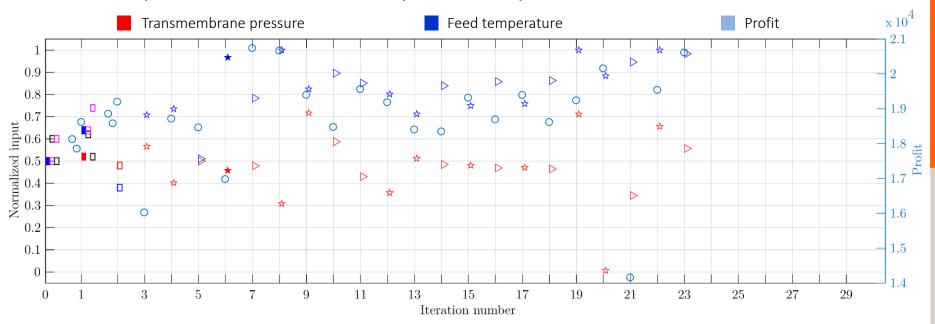


Figure: Experimental results for the unconstrained case: Evolution of the inputs (normalized) transmembrane pressure, temperature and the profit function obtained using process measurements. The tuning parameters  $\gamma$ ,  $\Delta u$ ,  $\Delta h$  and  $\delta$  were set to 3.0, 0.1, 0.1 and 0.1, respectively.



Motivation	Real-time optimization	Modifier adaptation with quadratic approximation (MAWQA)	Case study	Summary
0	0	0000	0 • 0 0	0
Experiment result: Unconstraine	ed case			

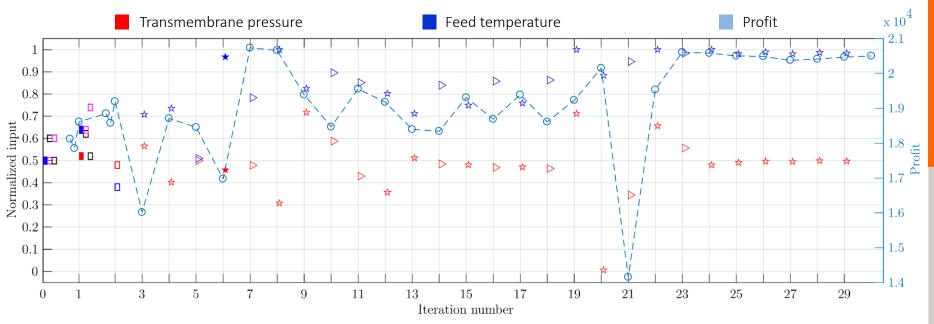


Figure: Experimental results for the unconstrained case: Evolution of the inputs (normalized) transmembrane pressure, temperature and the profit function obtained using process measurements. The tuning parameters  $\gamma$ ,  $\Delta u$ ,  $\Delta h$  and  $\delta$  were set to 3.0, 0.1, 0.1 and 0.1, respectively.

Motivation	Real-time optimization	Modifier adaptation with quadratic approximation (MAWQA)	Case study	Summary
0	0	0000	0000	0
Experiment result: Constrained	case			

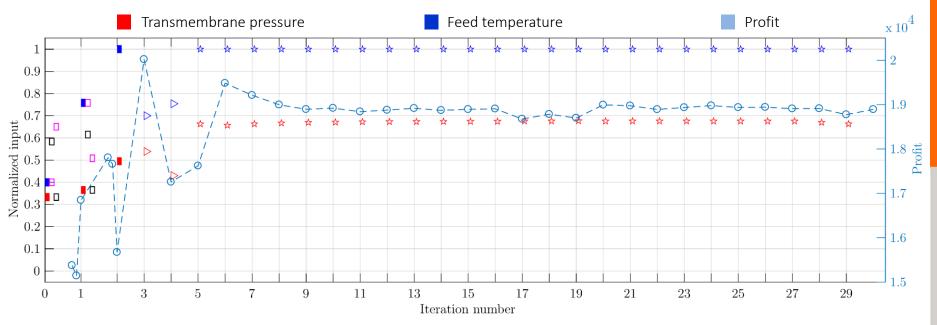
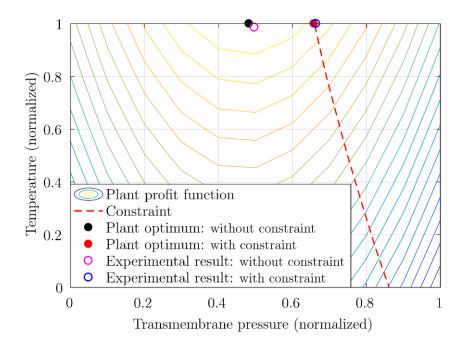


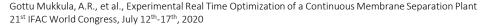
Figure: Experimental results for the constrained case: Evolution of the inputs (normalized) transmembrane pressure, temperature and the profit function obtained using process measurements. The values of the tuning parameters  $\gamma$ ,  $\Delta u$ ,  $\Delta h$  and  $\delta$  used in the MAWQA scheme are set to 3.0, 0.25, 0.25 and 0.25.

Motivation	Real-time optimization	Modifier adaptation with quadratic approximation (MAWQA)	Case study	Summary
0	0	0000	000•	0
Validation				

### Validation of experiment results



Top figure: Contour plot of the profit function of the nominal models and of the plant, its optimum and the optimum identified by the MAWQA experiments for both the constrained and the unconstrained cases.



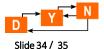


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Motivation	Real-time optimization	Modifier adaptation with quadratic approximation (MAWQA)	Case study	Summary
0	0	0000	0000	•
Summary & Outlook				

## Summary & Outlook

- We reported the development of an online real-time optimization solution (MAWQA) for the optimal operation of a continuously operated membrane plant with a nanofiltration membrane.
- Two experiments, one without constraints and another one with a productivity constraint were performed.
- In both experiments, the MAWQA scheme converged to an input close to the plant optimum that is predicted by the surrogate model for a large data set.
- The experiments validated that the combination of the plant measurements with MAWQA can drive a real plant to an optimal operation despite plant-model mismatch
- In our future work, we will focus on reducing the inefficient input moves and on developing a standardized approach for choosing the tuning parameters.



Motivation	Real-time optimization	Modifier adaptation with quadratic approximation (MAWQA)	Case study	Summary
0	0	0000	0000	0

# Thank you



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