Real-time optimization of a novel hydroformylation process by using transient measurements in modifier adaptation

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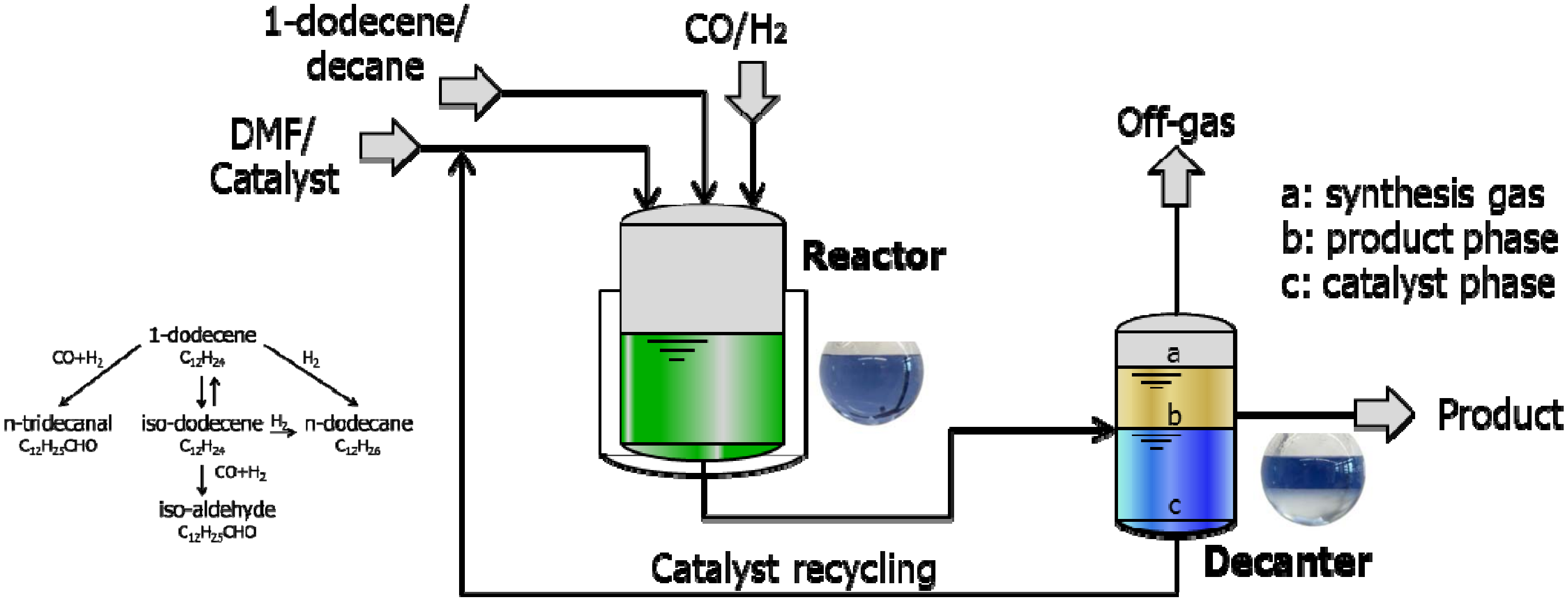
Outline

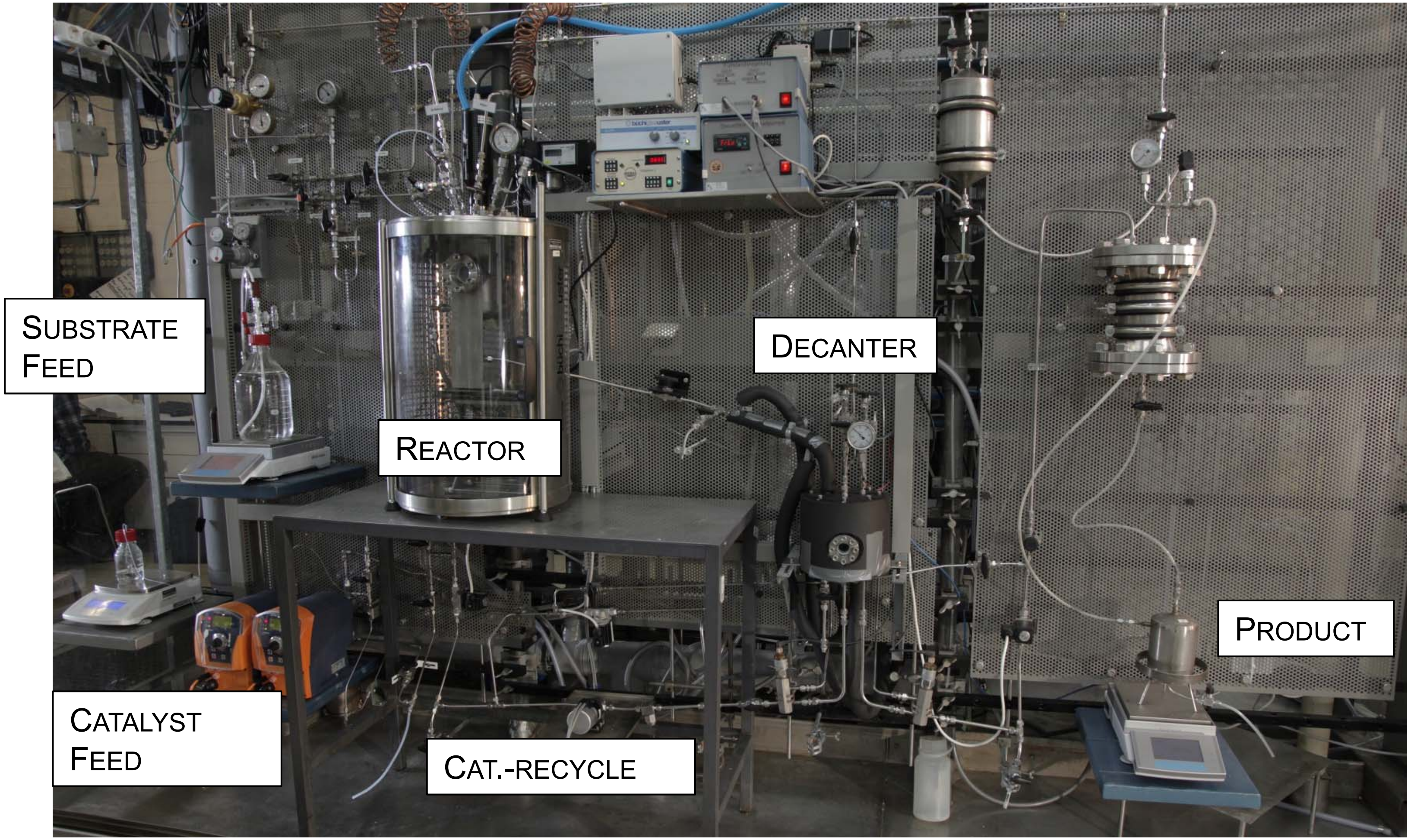
- Process description and optimization
- Handle model mismatch by modifier adaptation with quadratic approximation
  - Modifier adaptation optimization
  - Modifier adaptation with quadratic approximation
  - Compute steady state from transients
- Simulation study
- Summary

Hydroformylation of 1-dodecene



Temperature-controlled multicomponent solvent system

Miniplant operated at TUDO



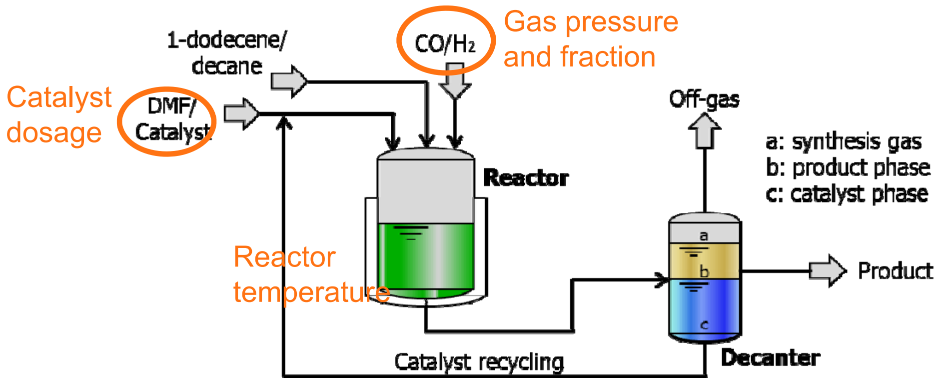
(Zagajewski et al., 2015)

Process Steady-state Optimization

Minimization of the operating cost per unit mass of tridecanal

$$\min_{u} \frac{Pr_{1-dodecene} \cdot F_{1-dodecene} + Pr_{Rh} \cdot F_{Rh} + C_{Cooling} + C_{Heating}}{F_{tridecanal}}$$

Steady-state mass flow of tridecanal



Mathematical modelling

Reactor part

$$V_R \frac{\mathrm{d}C_i}{\mathrm{d}t} = \dot{V}_{in} C_{i,in} - \dot{V}_{out} C_{i,out} + V_R C_{cat} M_{cat} \sum_{l=1}^{n_{react}} \nu_{i,l} r_l$$

$$V_R \frac{\mathrm{d}C_j}{\mathrm{d}t} = -k_{eff}(C_j - C_j^{eq}) + \dot{V}_{in} C_{j,in} - \dot{V}_{out} C_{j,out} + V_R C_{cat} M_{cat} \sum_{l=1}^{n_{react}} \nu_{j,l} r_l$$

$$C_j^{eq} = \frac{P_j}{H_{j,0} \exp\left(-E_j/RT\right)} \qquad C_{cat} = \frac{C_{Rh,precursor}}{1 + K_{cat,1} C_{CO} + K_{cat,2} C_{CO}/C_{H_2}}$$

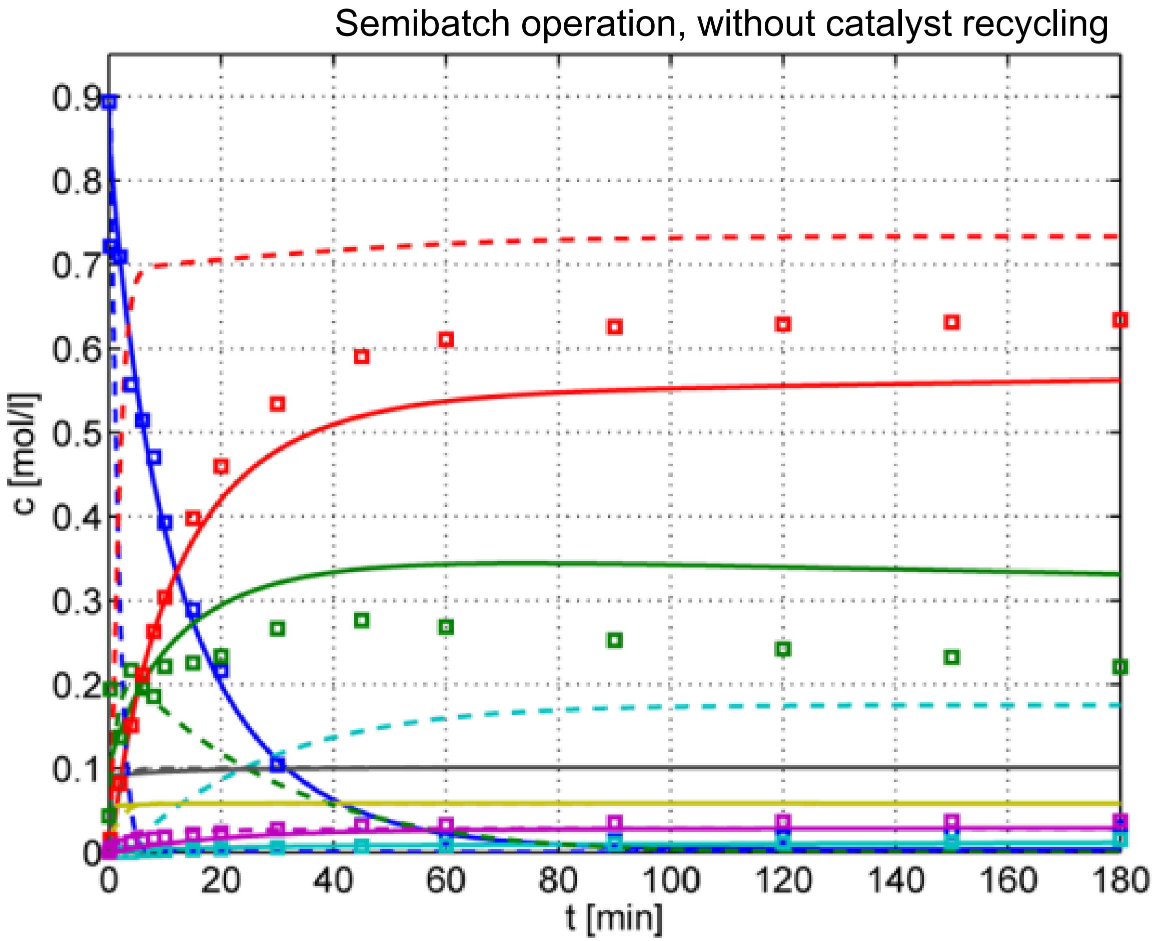
Decanter part

$$n_{i,product} = \frac{K_i}{1+K_i} n_{i,decanter} \qquad n_{i,catalyst} = \frac{1}{1+K_i} n_{i,decanter}$$

$$K_i = \exp\left(A_{i,0} + \frac{A_{i,1}}{T_{decanter}} + A_{i,2} T_{decanter}\right)$$

(Schäfer et al. 2012, Hentschel et al. 2015)

Model Mismatch



Symbols: experimental data. Dashed lines: model prediction with original parameters. Solid lines: Model prediction with refined parameters (Hentsche et al., 2015)

Modifier Adaptation Optimization

Measurements of the optimized variables and of the constrained variables are used to **adapt the optimization** problem such that the result converges iteratively to the true optimum of the plant

Nominal problem:

$$\begin{aligned} \min_{\mathbf{u}} \quad & J_m(\mathbf{u}) \\ \text{s.t.} \quad & \mathbf{C}_m(\mathbf{u}) \leq \mathbf{0} \end{aligned}$$

Index *m*: Model
p: Plant

Modifier-adapted problem:

$$\begin{aligned} \min_{\mathbf{u}} \quad & \boxed{J_m(\mathbf{u})} + \left(\boxed{\nabla J_p^{(k)}} - \nabla J_m^{(k)}\right)^T \left(\mathbf{u} - \mathbf{u}^{(k)}\right) \\ \text{s.t.} \quad & \boxed{\mathbf{C}_m(\mathbf{u})} + \boxed{\mathbf{C}_p^{(k)}} - \mathbf{C}_m^{(k)} + \left(\boxed{\nabla \mathbf{C}_p^{(k)}} - \nabla \mathbf{C}_m^{(k)}\right)^T \left(\mathbf{u} - \mathbf{u}^{(k)}\right) \leq \mathbf{0} \end{aligned}$$

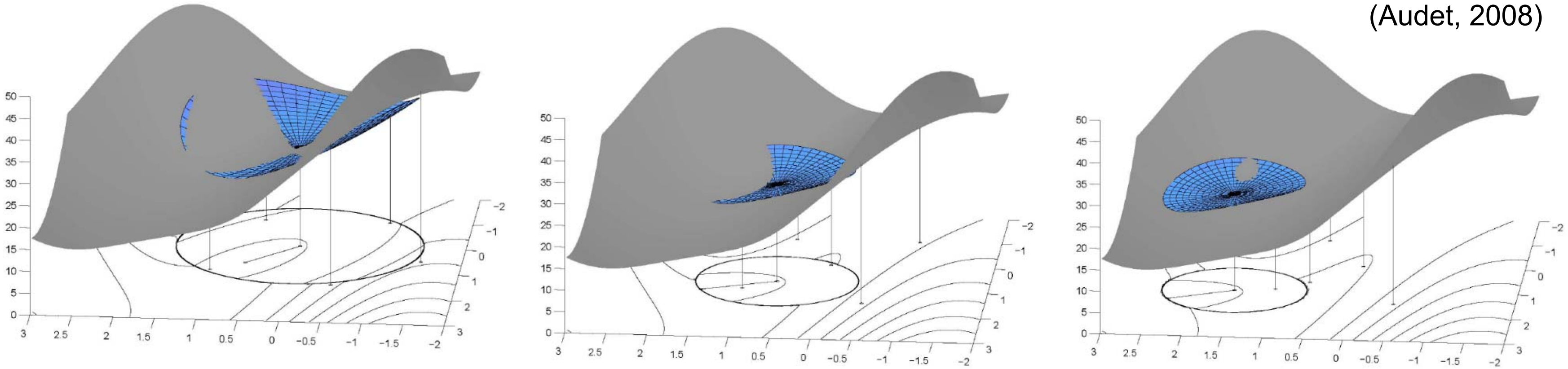
model adequacy

gradient estimation

(Gao and Engell 2005, Marchetti et al. 2009)

Quadratic Approximation Approach

(Audet, 2008)



- Optimization based upon probing of the target function and repeatedly constructing local quadratic functions
- Quadratic approximation enables the use of more distant points to decrease the influence of measurement noise

$$\min_{\mathbf{u}} \quad J_m(\mathbf{u}) + \left(\boxed{\nabla J_p^{(k)}} - \nabla J_m^{(k)}\right)^T \left(\mathbf{u} - \mathbf{u}^{(k)}\right)$$

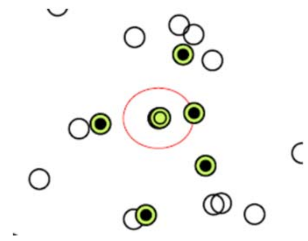
$$\text{s.t.} \quad \mathbf{C}_m(\mathbf{u}) + \mathbf{C}_p^{(k)} - \mathbf{C}_m^{(k)} + \left(\boxed{\nabla \mathbf{C}_p^{(k)}} - \nabla \mathbf{C}_m^{(k)}\right)^T \left(\mathbf{u} - \mathbf{u}^{(k)}\right) \leq \mathbf{0}$$

Gradients computed from the quadratic approximations

Modifer Adaptation with Quadratic Approximation

Integrate the second order information from the model with the gradient information from the quadratic approximation

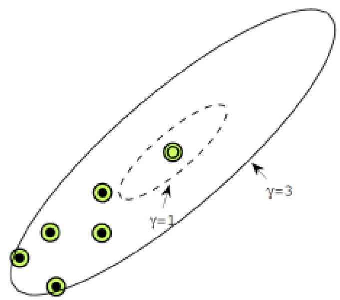
- Screen the collected data points to improve the quadratic approximations



- Monitor model quality and switch between modifier adaptation optimization and quadratic approximation optimization

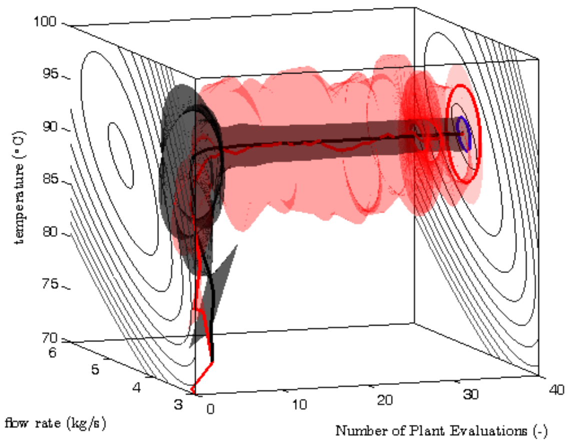
$$\begin{aligned} \min_{\mathbf{u}} \quad & J_{ad}^{(k)}(\mathbf{u}) \\ \text{s.t.} \quad & \mathbf{C}_{ad}^{(k)}(\mathbf{u}) \le 0 \\ & \mathbf{u} \in \mathcal{B}^{(k)} \end{aligned} \quad \longleftrightarrow \quad \begin{aligned} \min_{\mathbf{u}} \quad & J_{\phi}^{(k)}(\mathbf{u}) \\ \text{s.t.} \quad & \mathbf{C}_{\phi}^{(k)}(\mathbf{u}) \le 0 \\ & \mathbf{u} \in \mathcal{B}^{(k)} \end{aligned}$$

- Constraint the current search space to prevent too aggressive explorative moves

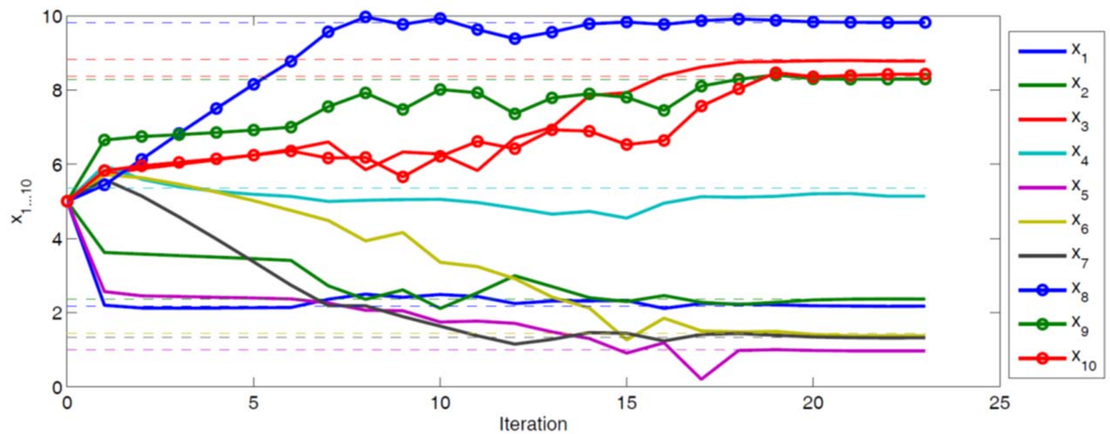


Modifier Adaptation with Quadratic Approximation

- Ensure convergence to the real optimum under considerable model mismatch
- Robust to measurement noise
- Efficient in term of number of plant evaluations



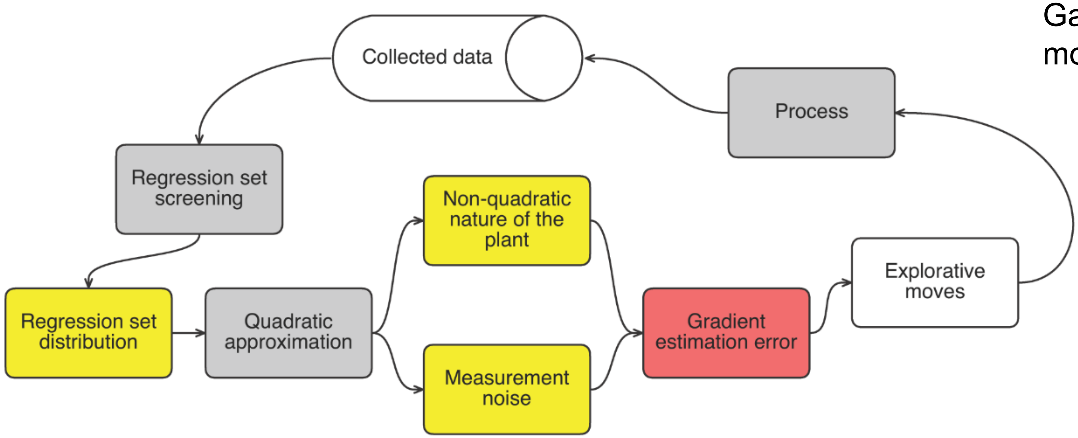
Mean and variance of the set-point trajectory for 100 realizations of the noise



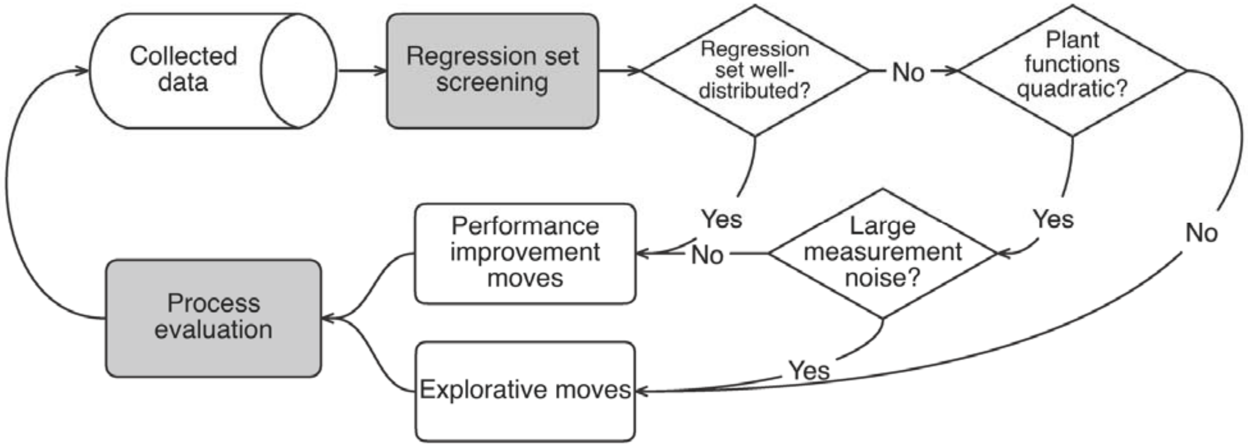
136 vs. 800 evaluations (algorithm based on fitting response surface, Caballero and Grossmann (2008))

W. Gao, S. Wenzel, S. Engell, A reliable modifier-adaptation strategy for real-time optimization. Computers & Chemical Engineering 2016 Best Paper Award

Explorative Moves in MAWQA

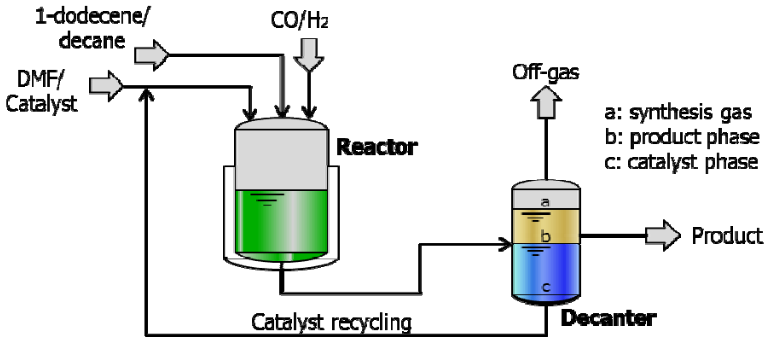


Gao et al. (2016) “A study of explorative moves during modifier adaptation with quadratic approximation”

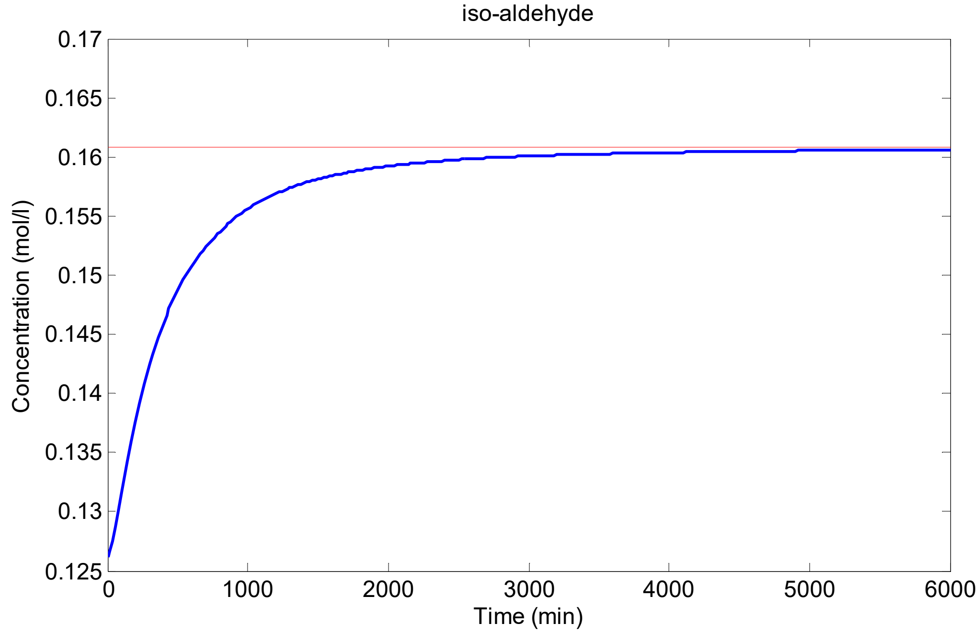


MAWQA algorithm takes only necessary explorative moves to improve the gradient estimations

Process with Slow Dynamics



Gas pressure change from 2 bar to 3 bar



Idea: react before settling to steady states

MA Approaches using Transients

- François and Bonvin (2014): Neighboring-extremal approach based on a variational analysis of the nominal model with respect to paramters and input variables

$$\boxed{\nabla_{\mathbf{u}} J(\mathbf{u},\theta)} \approx \nabla_{\mathbf{u}} J|_{\mathbf{u}_0,\theta_0} + \nabla^2_{\mathbf{uu}} J|_{\mathbf{u}_0,\theta_0} \Delta\mathbf{u} + \nabla^2_{\mathbf{u}\theta} J|_{\mathbf{u}_0,\theta_0} \boxed{\Delta\theta}$$

- Rodríguez-Blanco et al. (2017): Recursive extended least squares approach based on representing the dynamics of the cost function by a quadratic Taylor polynominal of the input variations (one formulation here)

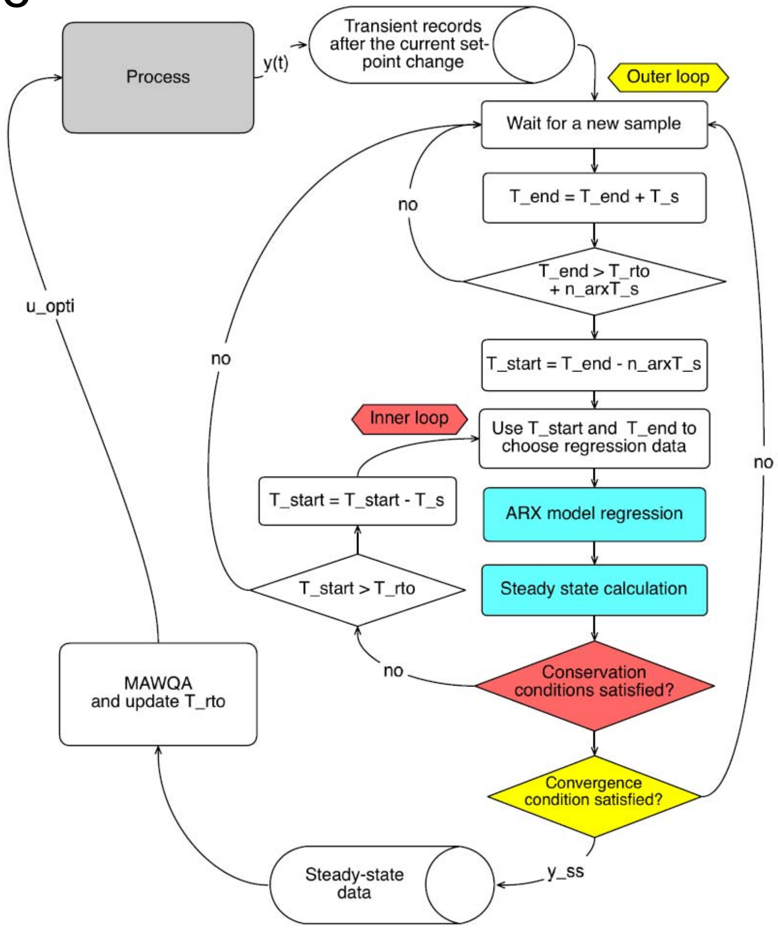
$$\boxed{\Delta\hat{J}_k} = \varphi_k^T \hat{\theta}_k = \boxed{\frac{\partial J}{\partial u_k}} \Delta u_k + \frac{\partial J}{\partial u_{k-1}} \Delta u_{k-1} + \frac{\partial^2 J}{\partial {u_k}^2} 1/2 \Delta {u_k}^2 + \frac{\partial^2 J}{\partial u_k u_{k-1}} \Delta u_k \Delta u_{k-1} + \frac{\partial^2 J}{\partial {u_{k-1}}^2} 1/2 \Delta {u_{k-1}}^2$$

Compute Steady State from Transients

Gao and Engell (2016) : Compute the next steady state from the transient response to the current set-point change

Assumption: The dynamics of the process can be approximated by a simple ARX model

- Determine the ARX model by a regression of the transients collected after the current set-point change
- Apply Limit Theorem to compute the next steady state
- Verify the computed steady state by
  - Conservation of mass and (or) energy at the predicted steady state
  - Convergence conditions: differences between two successive estimations are less than some threshold



Simulation Study

Transient records: concentrations of 1-dodecane, n-tridecanal, iso-dodecane, n-dodecane and iso-aldehyde in the production stream

Conservation condition:

$$\left|1-\frac{\dot{V}_{product}\left(C_{1,s}+C_{2,s}+C_{3,s}+C_{4,s}+C_{5,s}\right)}{\dot{V}_{in}C_{1,in}}\right|\leq 1e-3$$

Convergence condition:

$$\max\left(|\Delta C_{1,s}|,|\Delta C_{2,s}|,|\Delta C_{3,s}|,|\Delta C_{4,s}|,|\Delta C_{5,s}|\right)\leq 1e-3.$$

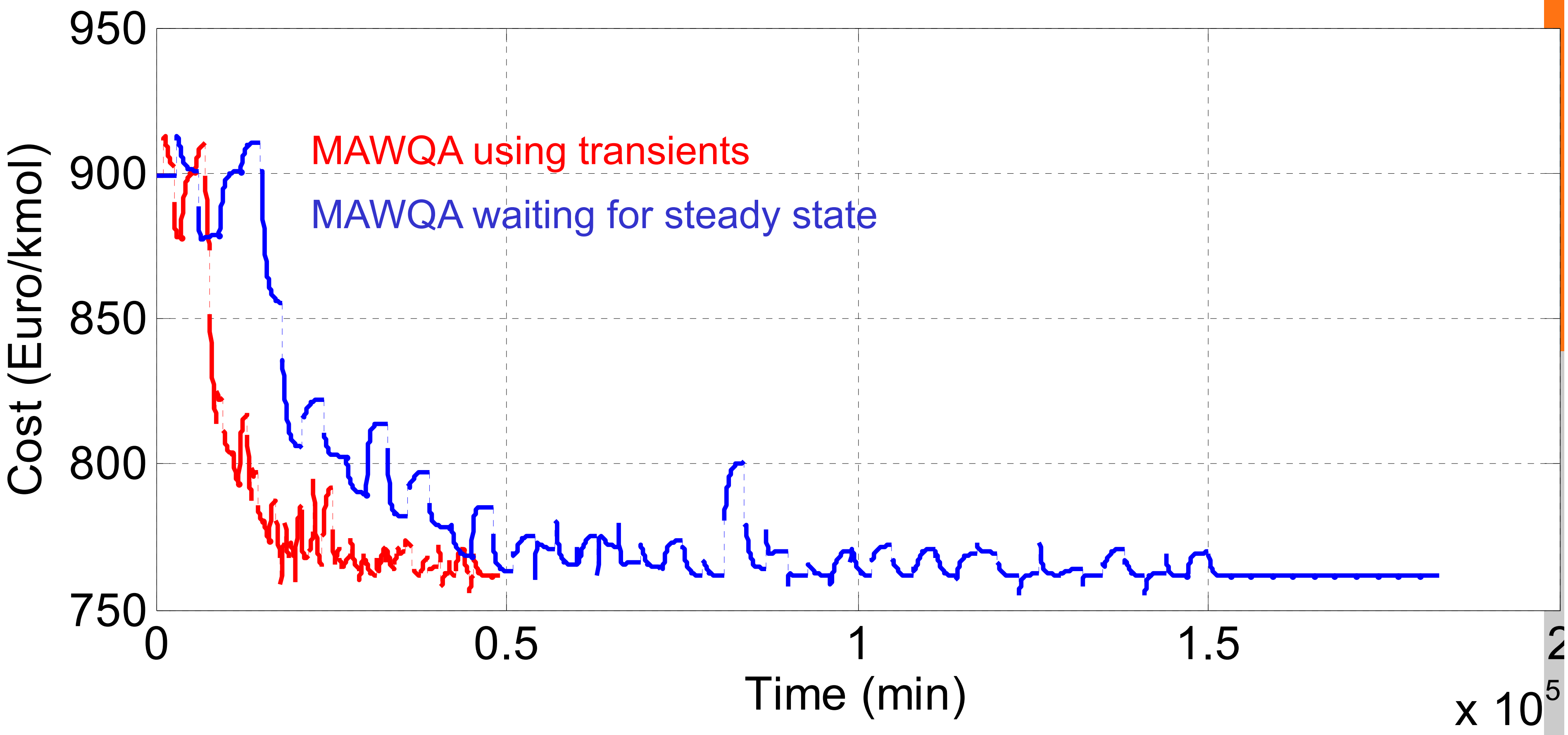
MAWQA based on a mismatched model:

$$C_j^{eq}=\frac{P_j}{\boxed{H_{j,0}}\exp\left(-E_j/RT\right)}$$

$$C_{cat}=\frac{C_{Rh,precursor}}{1+K_{cat,1}C_{CO}+\boxed{K_{cat,2}C_{CO}/C_{H_2}}}$$

	Operating interval	Initial set-point	Process optimum	MAWQA waiting for steady states	MAWQA using transients
Reactor temperature (°C)	85~105	95.0	88.64	88.78	89.07
Catalyst dosage (ppm)	0.25~2.0	1.1	0.51	0.52	0.49
Gas pressure (bar)	1.0~3.0	2.0	3.0	3.0	3.0
CO fraction	0.0~0.99	0.5	0.55	0.55	0.55
Cost (Euro/kmol)		899.04	761.33	761.33	761.43

Evolution of the cost function



Summary

- MAWQA: **Fast robust convergence** to the true plant optimum through the use of a **model of medium accuracy** and **measured data**
- Use of transients can accelerate the convergence to the optimal steady state
- Check of conservation and convergence conditions is necessary to ensure reasonable steady state estimation
- Current work:
  - Experimental test
  - Dual control – compromise between collecting useful information and optimizing the performance

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