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# Self-Optimizing Control in Chemical Recycle Processes

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**Abstract:** An engineer always has to make assumptions about the system boundary. In this paper, the impact of neglected dependencies of manipulated variables on the disturbance variables as example for said assumptions is investigated in the context of self-optimizing control. The feedback through dependent disturbances influences both the optimal operating point and the combination of measurements. As a case study, we consider an ammonia synthesis reactor with a simplified model for the ammonia separation and the recycle. The disturbance dependency changes the optimal selection matrices through the recycle. However, we find that it is possible to neglect the recycle in the selection of the controlled variables for this example if the setpoint is adjusted.



*Keywords:* Self-optimizing control, Integrated systems, Feedback through recycles, Control of ammonia reactors.

## 1. INTRODUCTION

Control structure design, and in particular what to control, is important for both economic performance and stabilization of a process. The aim of a good control structure is to operate at the economic optimum while satisfying safety and environmental constraints in the presence of disturbances. In order to achieve economic optimal operation, different methods can be utilized. One can generally distinguish between online and offline optimization methods. Examples for online optimization include real time optimization (RTO) and economic nonlinear model predictive control (E-NMPC), whereas offline methods include self-optimizing control (SOC).

The starting point for selecting a good control structure is to optimize the process for various disturbances. The aim is to find a simple way of implementing optimal operation, that is, a simple control structure with a small loss. Frequently, it is difficult to obtain a detailed process model that can be used for optimization, especially for systems that incorporate mass and energy recycles. In this situation, it may be possible to utilize the concepts of surrogate models to obtain such a process flowsheet (Straus and Skogestad, 2016), or use submodels in which optimization is applied locally.

Applying optimization locally, however, results in a scenario where the considered disturbances may be dependent on the selected input variables through the recycle, resulting in a feedback. Furthermore, the cost function may be different in the overall flowsheet and the submodels. The submodel operation point does not necessarily correspond to the true optimum including the recycle loop as well. Therefore, the application of self-optimizing control to individual submodels of a large process can result in a situation, in which the selected measurement combination is not optimal.

The aim of this paper is to investigate, how the dependency of disturbances may influence the theoretical performance of a self-optimizing control structure. Section 2 recapitulates SOC with focus on the applied exact local method (Halvorsen et al., 2003), whereas Section 3 looks into the effect of dependent disturbances in the calculation of the optimal selection matrix $\mathbf{H}$. Section 4 investigates the influence of the feedback on a case study representing an ammonia reactor with a simplified recycle loop.

## 2. SELF-OPTIMIZING CONTROL

Self-optimizing control (SOC) is the selection of controlled variables $\mathbf{c}$ which when kept constant in the case of a disturbance, result in an acceptable economic loss (Skogestad, 2000). The starting point is a steady-state optimization problem given by

$$\begin{aligned} \min_{\mathbf{x},\mathbf{u}} \quad & J(\mathbf{x},\mathbf{d},\mathbf{u}) \\ \text{s.t.} \quad & 0 = \mathbf{g}(\mathbf{x},\mathbf{d},\mathbf{u}) \\ & 0 \geq \mathbf{h}(\mathbf{x},\mathbf{d},\mathbf{u}) \end{aligned} \tag{1}$$

in which $\mathbf{x} \in \mathbb{R}^{n_x}$ denote the state variables, $\mathbf{d} \in \mathbb{R}^{n_d}$ the disturbance variables, and $\mathbf{u} \in \mathbb{R}^{n_u}$ the steady-state degrees of freedom. The process model itself is given by $\mathbf{g} : \mathbb{R}^{n_x} \times \mathbb{R}^{n_d} \times \mathbb{R}^{n_u} \rightarrow \mathbb{R}^{n_g}$ whereas $\mathbf{h} : \mathbb{R}^{n_x} \times \mathbb{R}^{n_d} \times \mathbb{R}^{n_u} \rightarrow \mathbb{R}^{n_h}$ denote the operational constraints given by the process. The cost function $J : \mathbb{R}^{n_x} \times \mathbb{R}^{n_d} \times \mathbb{R}^{n_u} \rightarrow \mathbb{R}$ describes an economic cost of the system.

For given disturbances $\mathbf{d}$, we assume that there exists an input $\mathbf{u}^{opt}(\mathbf{d})$ which minimizes the optimization problem (1). If different values than the optimal input $\mathbf{u}^{opt}$ are chosen for the manipulated variables $\mathbf{u}$, there will be a steady-state loss

$$L = J\left(\mathbf{u},\mathbf{d}\right) - J\left(\mathbf{u}^{opt}(\mathbf{d}),\mathbf{d}\right) \tag{2}$$

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The aim of self-optimizing control is then to find controlled variables $\mathbf{c}$ which when kept constant give a $\mathbf{u}$ that minimize this loss for expected disturbances.

One direct solution to self-optimizing control is to control the gradient of the cost function $J$ with respect to the inputs $\mathbf{u}$ ($\mathbf{J_u}$) to 0 as this would imply that the cost function is always at an extremum. The corresponding model-free approach of controlling the measured gradient to zero is called extremum seeking control and dates back to 1922 (Tan et al., 2010). However, in general, the gradient cannot be measured. In certain cases it is possible to express the gradient of the cost function as a direct function of the measurements and control it to 0 (Jäschke and Skogestad, 2014).

As it is frequently not possible to obtain the gradient of the cost function as a simple expression of the measurements $\mathbf{y} \in \mathbb{R}^{n_y}$

$$\mathbf{y} = \mathbf{h_y}(\mathbf{x}, \mathbf{d}, \mathbf{u}) \tag{3}$$

it is necessary to define the controlled variables $\mathbf{c}$ as a function of the available measurements as

$$\mathbf{c} = \mathbf{h_c}(\mathbf{y}) \tag{4}$$

in which $\mathbf{h_c} : \mathbb{R}^{n_y} \to \mathbb{R}^{n_c}$ may be a function of any type. Frequently, linear measurement combinations are used resulting in

$$\mathbf{c} = \mathbf{H}\mathbf{y} \tag{5}$$

in which $\mathbf{H} \in \mathbb{R}^{n_c \times n_y}$.

### *2.1 Linearization of the process model and cost function*

The majority of the self-optimizing control methods are based on a local analysis at the nominal optimal operation point. This results in a linearization of the measurements

$$\mathbf{y} = \mathbf{G^y}\mathbf{u} + \mathbf{G_d^y}\mathbf{d} \tag{6}$$

where $\mathbf{G^y} \in \mathbb{R}^{n_y \times n_u}$ and $\mathbf{G_d^y} \in \mathbb{R}^{n_y \times n_d}$ are the process and disturbance gain matrices, respectively. The cost is approximated through a second order Taylor expansion around the nominal operation point ($\mathbf{u}^*$, $\mathbf{d}^*$)

$$\begin{aligned} J(\mathbf{u}, \mathbf{d}) =& J(\mathbf{u}^*, \mathbf{d}^*) + \begin{bmatrix} \mathbf{J_u} \\ \mathbf{J_d} \end{bmatrix}^\mathsf{T} \begin{bmatrix} \Delta\mathbf{d} \\ \Delta\mathbf{u} \end{bmatrix} \\ &+ \frac{1}{2} \begin{bmatrix} \Delta\mathbf{d} \\ \Delta\mathbf{u} \end{bmatrix}^\mathsf{T} \begin{bmatrix} \mathbf{J_{uu}} & \mathbf{J_{ud}} \\ \mathbf{J_{ud}^\mathsf{T}} & \mathbf{J_{dd}} \end{bmatrix} \begin{bmatrix} \Delta\mathbf{d} \\ \Delta\mathbf{u} \end{bmatrix} \end{aligned} \tag{7}$$

with $\Delta\mathbf{d} = \mathbf{d} - \mathbf{d}^*$ and $\Delta\mathbf{u} = \mathbf{u} - \mathbf{u}^*$. Note, that the derivatives $\mathbf{J_u}$, $\mathbf{J_d}$, $\mathbf{J_{uu}}$, $\mathbf{J_{ud}}$, and $\mathbf{J_{dd}}$ are evaluated at the nominal point ($\mathbf{u}^*$, $\mathbf{d}^*$). Combining (2) with (7) and utilizing that $\mathbf{J_u} = 0$ at the optimum, we can calculate the loss for disturbances $\mathbf{d} = \mathbf{d}^*$ as

$$L = \frac{1}{2} \left(\mathbf{u} - \mathbf{u}^{opt}(\mathbf{d})\right)^\mathsf{T} \mathbf{J_{uu}} \left(\mathbf{u} - \mathbf{u}^{opt}(\mathbf{d})\right) \tag{8}$$

### *2.2 Calculation of the selection matrix* $\mathbf{H}$

Several methods exist to obtain optimal measurement combinations, $\mathbf{c} = \mathbf{H}\mathbf{y}$. The reader is referred to (Jäschke et al., 2017) for a concise review of the different methods which can be utilized. In this study, the exact local method as developed by Halvorsen et al. (2003) and simplified by Yelchuru and Skogestad (2012) is utilized. In order to make a statement about the loss, Halvorsen et al. (2003) introduced diagonal scaling matrices for the disturbances $\mathbf{W_d}$ and measurement errors $\mathbf{W_{n^y}}$ as

$$\Delta\mathbf{d} = \mathbf{W_d}\mathbf{d}'; \qquad \mathbf{n^y} = \mathbf{W_{n^y}}\mathbf{n^{y'}} \tag{9}$$

in which the vectors $\mathbf{d}'$ and $\mathbf{n^{y'}}$ are assumed to satisfy

$$\left\| \begin{bmatrix} \mathbf{d}' \\ \mathbf{n^{y'}} \end{bmatrix} \right\|_2 \leq 1 \tag{10}$$

For a given selection matrix $\mathbf{H}$, the linearized model (6), and the general loss expression (8), it is possible to derive the worst-case loss (Halvorsen et al., 2003) and the average expected loss (Kariwala et al., 2008) as

$$L_{WC}(\mathbf{H}) = \frac{1}{2}\bar{\sigma}(\mathbf{M})^2 \tag{11}$$

$$L_{avg}(\mathbf{H}) = \frac{1}{2}\|\mathbf{M}\|_F^2 \tag{12}$$

in which the loss matrix $\mathbf{M}$ is shown to be

$$\mathbf{M} = \mathbf{J_{uu}}^{1/2} (\mathbf{H}\mathbf{G^y})^{-1} \mathbf{H}\mathbf{Y} \tag{13}$$

with

$$\mathbf{Y} = [\mathbf{F}\mathbf{W_d} \ \mathbf{W_{n^y}}] \tag{14}$$

The optimal sensitivity matrix for the measurements $\mathbf{F}$ can be obtained numerically or calculated from the linearized model (Halvorsen et al., 2003)

$$\mathbf{F} = \frac{\partial \mathbf{y}^{opt}}{\partial \mathbf{d}} \tag{15}$$

$$= -\left(\mathbf{G^y}\mathbf{J_{uu}^{-1}}\mathbf{J_{ud}} - \mathbf{G_d^y}\right) \tag{16}$$

The optimal measurement combination $\mathbf{H}$ can now be calculated as the solution which minimizes the average (12) and worst case (11). Both these optimization problems have the same optimal solution (Kariwala et al., 2008) which can be obtained by solving

$$\min_{\mathbf{H}} \left\| \mathbf{J_{uu}}^{1/2} (\mathbf{H}\mathbf{G^y})^{-1} \mathbf{H}\mathbf{Y} \right\|_F \tag{17}$$

The analytical solution to this problem was first described by Alstad et al. (2009) and later simplified by Yelchuru and Skogestad (2012) to

$$\mathbf{H}^\mathsf{T} = \left(\mathbf{Y}\mathbf{Y}^\mathsf{T}\right)^{-1} \mathbf{G^y} \tag{18}$$

From (18) and (14), we can see that the required model information is $\mathbf{G^y}$ and $\mathbf{F}$, where the latter can be calculated using (16). In practice, if a nonlinear process model is utilized, it is simpler to calculate $\mathbf{F}$ numerically from (15). Similarly, the loss $L$ can be calculated using the nonlinear model and optimization problem (1).

## 3. DEPENDENT DISTURBANCES

Consider the block diagram in Figure 1, where "Local plant" represents our submodel (ammonia reactor in our case study) and "Remaining plant" represents the neglected part of the process (the recycle in our case).

The first question now is: Assume that we optimize our "Local plant" with a fixed value of $\mathbf{d}_0$, that is, we neglect the effect $\mathbf{u}$ has on $\mathbf{d}_0$ through, for example, the recycle. Is this acceptable? Of course, the answer is generally no

The second question is: Assume now that we find controlled variables (that is, find $\mathbf{H}_0$) based on considering our "Local plant". Is this acceptable? Again, the answer is generally no, but in practice the answer may be "yes" if the local cost function is the same as the overall one. To

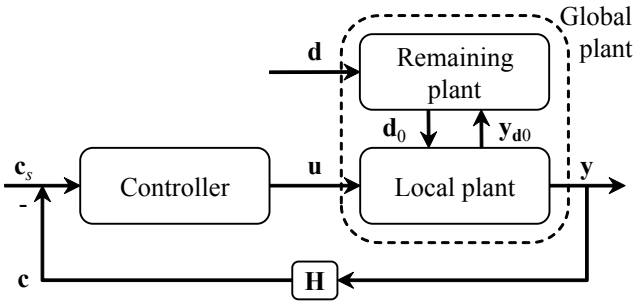


Fig. 1. Visualization of the dependency of local disturbances $\mathbf{d}_0$ on the inputs $\mathbf{u}$, measurements $\mathbf{y}$, and the independent disturbances $\mathbf{d}$.

better understand this, let us consider how the matrices used to find $\mathbf{H}$ in (13) and (14) may change.

To see the difference between $\mathbf{G}^{\mathbf{y}}$ (based on the overall plant) and $\mathbf{G}_0^{\mathbf{y}}$ (based on the local plant), we can look at the total differential,

$$\begin{aligned}\mathbf{G}^{\mathbf{y}} &\triangleq \left(\frac{\mathrm{d}\mathbf{y}}{\mathrm{d}\mathbf{u}}\right)_{\mathbf{d}} \\ &= \left(\frac{\partial \mathbf{y}}{\partial \mathbf{u}}\right)_{\mathbf{d}_0} + \frac{\partial \mathbf{y}}{\partial \mathbf{d}_0}\frac{\partial \mathbf{d}_0}{\partial \mathbf{y}_{\mathbf{d}0}}\frac{\mathrm{d}\mathbf{y}_{\mathbf{d}0}}{\mathrm{d}\mathbf{u}} \\ &= \mathbf{G}_0^{\mathbf{y}} \quad + \mathbf{G}_{\mathbf{d}0}^{\mathbf{y}}\,\mathbf{G}_{\mathbf{y}_{\mathbf{d}0}}^{\mathbf{d}0}\,\mathbf{G}_{\mathbf{u}}^{\mathbf{y}_{\mathbf{d}0}}\end{aligned} \tag{19}$$

with $\mathbf{y}_{d0}$ corresponding to the outlet variables of the local plant which affect the neglected part, see Figure 1. In our case, these are the outlet flow, pressure, temperature, and composition. The gain $\mathbf{G}_{\mathbf{y}_{\mathbf{d}0}}^{\mathbf{d}0}$ is the previously neglected feedback and can be obtained from the submodel of the remaining plant. The gain $\mathbf{G}_{\mathbf{u}}^{\mathbf{y}_{\mathbf{d}0}}$ corresponds to the change in the outlet variables with changing input.

A similar analysis can be conducted for the Hessian of the cost function ($\mathbf{J}_{\mathbf{uu}}$) and the disturbance gain $\mathbf{G}_{\mathbf{d}}^{\mathbf{y}}$.

## 4. CASE STUDY - AMMONIA SYNTHESIS LOOP

The core of the case study is a three-bed ammonia reactor previously described by Morud and Skogestad (1998) and utilized by Straus and Skogestad (2017) in the application of economic nonlinear model predictive control. In this model, the disturbances ($\mathbf{d}_0$) are the inlet variables to the system

$$\mathbf{d}_0 = [\dot{m}_{Feed0}\ p_{Feed0}\ T_{Feed0}\ w_{\mathrm{NH_3},Feed0}] \tag{20}$$

There exist 3 input variables ($\mathbf{u}$), which correspond to the split ratios to the three reactor beds. The cost function for the ammonia reactor is to maximize the extent of reaction $\xi$, *i.e.*

$$\begin{aligned}J &= -\xi \\ &= -\dot{m}_{Feed0}\left(w_{\mathrm{NH_3},Rea} - w_{\mathrm{NH_3},Feed0}\right)\end{aligned} \tag{21}$$

As the reaction is limited by the thermodynamical equilibrium, a recycle is necessary to utilize the unreacted hydrogen and nitrogen. The reactor is connected to the recycle through the inlet stream $\mathbf{d}_0$ and the outlet stream $\mathbf{y}_{\mathbf{d}0}$. This recycle stream ($\mathbf{d}_r$) corresponds to 75 % of the mass of the feed to the reactor. Hence, the impact of the dependency of the neglected remaining plant is expected to be large in this case study.

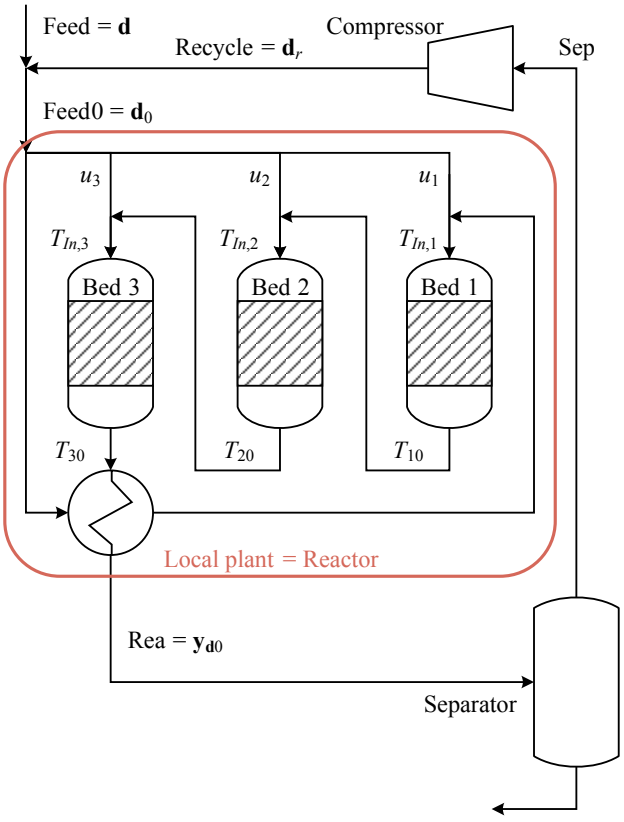


Fig. 2. Heat-integrated three-bed reactor system incorporated into a simple recycle system consisting of a separator and a recycle compressor.

The model incorporating the recycle is depicted in Figure 2. In the recycle system, the actual disturbances (which usually are the true disturbances) are the inlet values to the new system:

$$\mathbf{d} = [\dot{m}_{Feed}\ p_{Feed}\ T_{Feed}\ w_{\mathrm{NH_3},Feed}]^{\mathsf{T}} \tag{22}$$

Note, that $\mathbf{d}_0$ is dependent on both $\mathbf{d}$ and $\mathbf{y}_{\mathbf{d}0}$ (through $\mathbf{d}_r$) as fresh feed is mixed with the recycle.

### *4.1 Model description*

The recycle adds the following assumptions to the model in addition to the ones described previously:

- hydrogen and nitrogen are fed as a stoichiometric mixture and no inerts are present in the feed, resulting in neglecting a purge flow;
- the feed to the system determines the pressure in the reactor as well as the inlet temperature of the reactor system;
- the pressure drop in the system occurs after the reactor resulting in a constant pressure in the reactor;
- the compressor operates with a fixed efficiency of $\eta = 80$ % and is considered to be isothermal as the compression ratio is smaller than 1.1 in an ammonia synthesis loop;
- the separation is defined *via* a (fixed) separation coefficient $\alpha = 0.25$ and only ammonia is separated.

Based on the assumptions, the separation of ammonia is then calculated as

$$\dot{m}_{Sep} w_{\mathrm{NH_3},Sep} = \alpha \dot{m}_{Rea} w_{\mathrm{NH_3},Rea} \tag{23}$$

Table 1. Nominal (optimal) inlet conditions for the reactor

| Recycle | $\dot{m}_{Feed0}$ [kg/s] | $p_{Feed0}$ [bar] | $T_{Feed0}$ [°C] | $w_{\mathrm{NH_3},Feed0}$ [wt.%] |
|---|---|---|---|---|
| Without | 70.0 | 200 | 250 | 8.0 |
| With | 61.8 | 200 | 250 | 8.3 |

Additionally, a model equation similar to a valve coefficient has to be added for the pressure drop after the separator

$$0 = \dot{n}_{Sep} - k\sqrt{p_{Feed} - p_{Sep}} \tag{24}$$

with a given pressure drop coefficient $k$ ($\mathrm{kmol}/(\mathrm{s}\cdot\sqrt{\mathrm{bar}})$). The compressor duty of an isothermal compressor is (*e.g.* Skogestad (2008))

$$W = \frac{\dot{n}_{Sep} R T_{Feed}}{\eta} \ln\left(\frac{p_{Feed}}{p_{Sep}}\right) \tag{25}$$

As there is no purge flow and the product is pure ammonia, all of the feed has to be converted. The system will therefore operate with a constant extent of reaction, and hence, it cannot be used anymore as cost function as it was the case in the local reactor system. Instead, the new economic cost function corresponds to minimizing the compressor duty of the recycle loop, *i.e.*

$$J = W \tag{26}$$

As mentioned beforehand, this change in cost function may affect SOC variables defined for the reactor system. The new cost function aims at minimizing the flow within the recycle. This corresponds to minimizing the feed flow to the reactor while maintaining a constant extent of reaction. It can be seen as equivalent to the old cost function where the aim is to maximize the extent of reaction for a given feed. Alternatively, maximizing the conversion *per pass* can be used in both cases as it is equivalent to $\xi$ for a fixed feed and in addition minimize the recycle flow.

The optimization was performed using CasADi (Andersson, 2013) with IPOPT (Wächter and Biegler, 2006).

Let us first consider the first question in Section 3; is it possible to optimize the reactor neglecting the recycle? With the new cost function and the modified system, the optimal nominal inlet conditions of the reactor are given in Table 1. Unsurprisingly, it is not possible to neglect the recycle in the optimization. Especially the reactor inlet mass flow $\dot{m}_{Feed0}$ changes a lot due to the recycle. This is caused by a positive feedback. A higher conversion *per pass* corresponds to more ammonia separated, and hence, a lower recycle flowrate. This in turn increases the residence time in the beds and hence increases the conversion *per pass*. The ammonia mass fraction experiences negative feedback due to the assumption of a constant split factor. Hence, its value changes only by a small value. Due to the aforementioned assumptions, the inlet pressure and temperature of the system are the same with and without the recycle stream.

### *4.2 Application of SOC*

This brings us to the second question in Section 3. Are the controlled variables $\mathbf{c}_0 = \mathbf{H}_0\mathbf{y}$ based on considering only the reactor a valid choice?

To this end, we apply the exact local method as explained in Section 2.2 to both only the reactor (local plant) and to the reactor+recycle (global plant). In order to reduce the number of measurements utilized and pair the controlled variables close to the inputs, each reactor bed is treated individually and the exact local method is applied to the inlet temperature and the outlet temperature of the respective reactor bed; *i.e.*

$$\mathbf{y}_i = \begin{bmatrix} T_{In,i} \\ T_{i0} \end{bmatrix} \qquad \forall i = 1,2,3 \tag{27}$$

This results in the combination of two measurements and corresponds additionally to selecting measurements that have a high gain from the input to the respective measurements.

The scaling matrices for the disturbance and measurement error in (9) are given by

$$\mathbf{W_d} = \mathrm{diag}\left([5\ \ 20\ \ 20\ \ 1]\right) \tag{28}$$

$$\mathbf{W}_{\mathbf{n}^\mathbf{y},i} = \mathrm{diag}\left([4\ \ 4]\right) \qquad \forall i = 1,2,3 \tag{29}$$

This implies that the actual optimal operation point with recycle does not fulfill requirement (10).

Utilizing the initial model of the reactor without recycle and cost function (21), we achieve the following combinations of self-optimizing control variables ($\mathbf{H}_0$)

$$\begin{aligned} c_{1,0} &= 0.053\ T_{In,1} + T_{10} \\ c_{2,0} &= 0.329\ T_{In,2} + T_{20} \\ c_{3,0} &= 1.311\ T_{In,3} + T_{30} \end{aligned} \tag{30}$$

whereas, if we incorporate the recycle in the calculation of our SOC variables and use cost function (26), we get ($\mathbf{H}$)

$$\begin{aligned} c_1 &= -0.288\ T_{In,1} + T_{10} \\ c_2 &= -0.161\ T_{In,2} + T_{20} \\ c_3 &= \ \ 0.940\ T_{In,3} + T_{30} \end{aligned} \tag{31}$$

Comparing (30) and (31), we can directly see that there are changes in the SOC variables. The most important measurement ($T_{10}$, $T_{20}$) in the first 2 self-optimizing variables $c_i$ remains the same, however the weights change.

This can be partly explained by an increase in the process gains $\mathbf{G}_1^\mathbf{y}$, $\mathbf{G}_2^\mathbf{y}$, and $\mathbf{G}_3^\mathbf{y}$ corresponding to the gains from $u_i$ to $\mathbf{y}_i$ by around 15% in average:

$$\begin{aligned} \mathbf{G}_{1,0}^\mathbf{y} &= -\begin{bmatrix} 576 \\ 1071 \end{bmatrix}, & \mathbf{G}_1^\mathbf{y} &= -\begin{bmatrix} 667 \\ 1283 \end{bmatrix} \\ \mathbf{G}_{2,0}^\mathbf{y} &= -\begin{bmatrix} 603 \\ 800 \end{bmatrix}, & \mathbf{G}_2^\mathbf{y} &= -\begin{bmatrix} 703 \\ 948 \end{bmatrix} \\ \mathbf{G}_{3,0}^\mathbf{y} &= -\begin{bmatrix} 563 \\ 229 \end{bmatrix}, & \mathbf{G}_3^\mathbf{y} &= -\begin{bmatrix} 656 \\ 253 \end{bmatrix} \end{aligned} \tag{32}$$

The changes in the optimal sensitivity matrices $\mathbf{F}_i$ (not shown) are even more pronounced, especially for the two disturbances with different values in the nominal optimal case; the inlet flowrate $\dot{m}_{Feed0}$ ($\dot{m}_{Feed}$) and the inlet mass fraction $w_{\mathrm{NH_3},Feed0}$ ($w_{\mathrm{NH_3},Feed}$).

Based on these findings, it can be concluded that the linearization (not surprisingly) looses validity through the introduction of a recycle stream. This can be caused by the change in the optimal inlet flowrate of the reactor as shown in Table 1. $\dot{m}_{Feed0}$ is reduced by 12 % and should be outside the linear range of the nonlinear model.

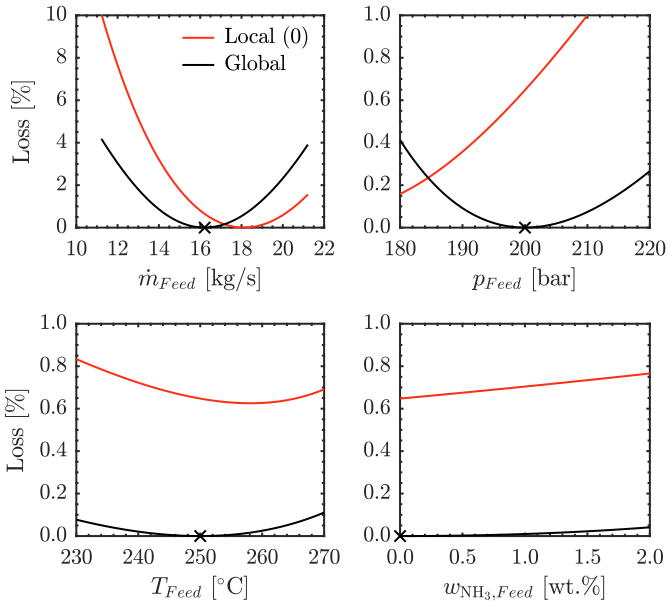


Fig. 3. Loss as a function of the disturbance for both cases ($\mathbf{H}_0$ and $\mathbf{H}$). The setpoints for the local selection matrices $\mathbf{H}_{i,0}$ are not adjusted to optimal setpoints of the global recycle system.

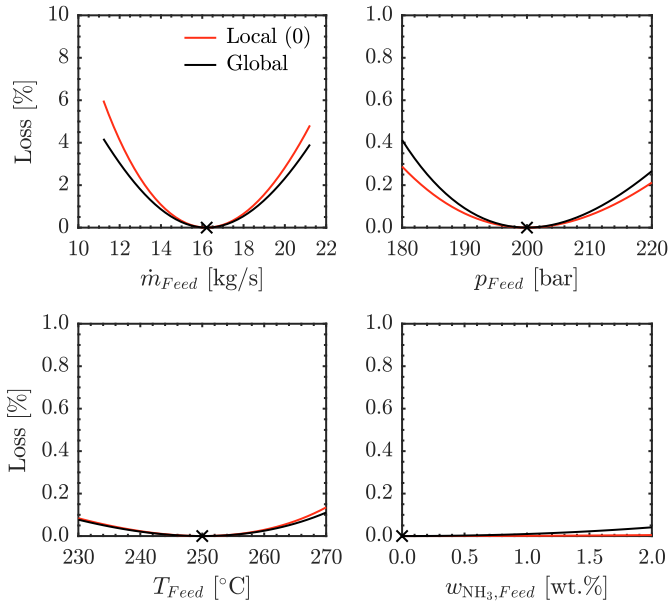


Fig. 4. Loss as a function of the disturbance for both cases ($\mathbf{H}_0$ and $\mathbf{H}$). The setpoints for local selection matrices $\mathbf{H}_{i,0}$ are adjusted to optimal setpoints of the global recycle system.

Adjusting the reactor inlet in the model without recycle to the new optimal value allows the verification of this claim. The plant gains $\mathbf{G}_i^{\mathbf{y}}$ are in this situation similar to the ones with recycle. Furthermore, $\mathbf{J_{uu}}$ is similar except for a scalar multiplier. This can be explained by the total differential (19). In the case of the ammonia reactor with a maximized extent of reaction, $w_{\mathrm{NH_3},Rea}$ is maximized. In addition, $T_{Rea}$ is maximized as well whereas $p_{Rea}$ and $\dot{m}_{Rea}$ are unaffected due to mass conservation and the assumption of constant feed pressure to the reactor. Hence, in our case $\mathbf{G}_{\mathbf{u}}^{\mathbf{y_{d0}}} = 0$ and

$$\mathbf{G}^{\mathbf{y}} = \mathbf{G}_0^{\mathbf{y}} \tag{33}$$

This special behaviour occurs, if the outlet variables are equivalent to the cost function.

The optimal sensitivity matrices change however due the neglected dependency of $\mathbf{d}_0$ on $\mathbf{y_{d0}}$ (and hence $\mathbf{u}$) through changes in $\mathbf{G}_{\mathbf{d}}^{\mathbf{y}}$ and $\mathbf{J_{ud}}$. This explains the changes in the selection matrices $\mathbf{H}_i$, see (30) and (31).

### *4.3 Loss calculation*

In order to evaluate the performance of both CV selections, $\mathbf{H}_{i,0}$ in (30) and $\mathbf{H}_i$ in (31), the loss as defined in (2) with the cost function (26) and the (nonlinear) model including the recycle was calculated. The setpoints for the controller in the problem without recycle were given by the optimal setpoints without recycle. The comparison of both losses is shown in Figure 3. As can be seen from the red curves in Figure 3, there is a loss even at the nominal point. This is not necessarily caused by a poor $\mathbf{H}_0$ matrix, but by a non-optimal operating point.

Hence, the setpoint for the SOC variables should be adjusted to the new nominal optimum in which the recycle is considered. The new loss calculations are shown in Figure 4. It is interesting to note, that the differences are surprisingly small. For an inlet pressure disturbance and mass flow disturbance, the loss is smaller for $\mathbf{H}$, whereas the loss is higher for $\mathbf{H}$ than for $\mathbf{H}_0$ for an inlet pressure and ammonia mass fraction disturbance.

Both $\mathbf{H}_0$ and $\mathbf{H}$ use the same weighting matrices (9). As the reactor inlet mass flow $\dot{m}_{Feed0}$ is varying between 42 kg/s and 84 kg/s for a flowrate disturbance, we can directly see the incorrect weighting of the inlet mass flow. Changing the value of the mass flow disturbance in the weighting matrix to 20 kg/s results in new controlled variables ($\mathbf{H}_{0,2}$)

$$\begin{aligned} c_{1,0,2} &= -0.181\ T_{In,1} + T_{10} \\ c_{2,0,2} &= -0.053\ T_{In,2} + T_{20} \\ c_{3,0,2} &= \ \ 0.971\ T_{In,3} + T_{30} \end{aligned} \tag{34}$$

which are more similar to (31). The corresponding loss is depicted in Figure 5. We can directly see that the difference in the loss is marginal, especially for $\dot{m}_{Feed}$, which had the largest loss in Figure 4. This is not surprising as the the optimal selection matrix $\mathbf{H}_{0,2}$ (34) is close to $\mathbf{H}$ (31).

### *4.4 Discussion*

It has to be highlighted that in this specific case study, it was possible to define a cost function in the system without recycle which corresponds to the cost function in the system with recycle. This is not necessarily the case for all submodels of recycle systems. If one would consider the case of a detailed separation section, the aim would be to minimize the cooling costs for a given feed. This feed would also represent some of the disturbances to the model. An unconstrained optimal solution would be given by no cooling and hence no separation. Therefore, separation requirements are needed, either on the separated product or through assigning cost values to all connection streams. Hence, the optimal point would be based on these separation requirements. On the other hand, the

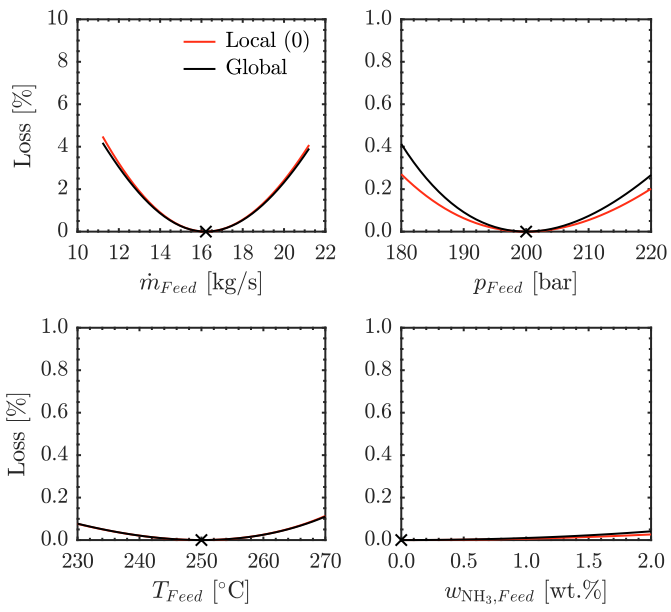


Fig. 5. Loss as a function of the disturbance for both cases ($\mathbf{H}_{0,2}$ and $\mathbf{H}$). The setpoints for local selection matrices $\mathbf{H}_{i,0,2}$ are adjusted to optimal setpoints of the global recycle system and the weighting matrix $\mathbf{W_d}$ changed.

total model does not need constraints on the separation as separating no product would result in no profit.

From the definition of the loss in (2), it is obvious that there is a constant loss at the nominal operation point if the setpoint for the self-optimizing variables is not adjusted. Recall that the starting point of this investigation is that it is however too complicated to optimize the overall model, and hence, to calculate the true optimal setpoint. Therefore, a model-free approach, *e.g.* extremum-seeking control or necessary conditions of optimality tracking (François et al., 2005), should be used on top of self-optimizing control for calculating the optimal setpoint.

## 5. CONCLUSION

The dependency of considered disturbances on the input (and measurements) changes the optimal selection matrix in the application of self-optimizing control. This is the case even if the actual values of the disturbances, and hence, the feed to the submodel are unchanged.

The loss is in the investigated case study similar if the setpoints to the controllers and the disturbance weighting matrix $\mathbf{W_d}$ are adjusted. This cannot be generalized and is depending on the neglected dependencies.

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## REFERENCES

Alstad, V., Skogestad, S., and Hori, E.S. (2009). Optimal measurement combinations as controlled variables. *Journal of Process Control*, 19(1), 138 – 148.

Andersson, J. (2013). *A General-Purpose Software Framework for Dynamic Optimization*. PhD thesis, Arenberg Doctoral School, KU Leuven, Department of Electrical Engineering (ESAT/SCD) and Optimization in Engineering Center, Kasteelpark Arenberg 10, 3001-Heverlee, Belgium.

François, G., Srinivasan, B., and Bonvin, D. (2005). Use of measurements for enforcing the necessary conditions of optimality in the presence of constraints and uncertainty. *Journal of Process Control*, 15(6), 701 – 712.

Halvorsen, I.J., Skogestad, S., Morud, J.C., and Alstad, V. (2003). Optimal selection of controlled variables. *Industrial & Engineering Chemistry Research*, 42(14), 3273–3284.

Jäschke, J., Cao, Y., and Kariwala, V. (2017). Self-optimizing control – a survey. *Annual Reviews in Control*, 43(Supplement C), 199 – 223.

Jäschke, J. and Skogestad, S. (2014). Optimal operation of heat exchanger networks with stream split: Only temperature measurements are required. *Computers & Chemical Engineering*, 70(Supplement C), 35 – 49. Manfred Morari Special Issue.

Kariwala, V., Cao, Y., and Janardhanan, S. (2008). Local self-optimizing control with average loss minimization. *Industrial & Engineering Chemistry Research*, 47(4), 1150–1158.

Morud, J.C. and Skogestad, S. (1998). Analysis of instability in an industrial ammonia reactor. *AIChE Journal*, 44(4), 888–895.

Skogestad, S. (2008). *Chemical and Energy Process Engineering*. CRC Press.

Skogestad, S. (2000). Plantwide control: the search for the self-optimizing control structure. *Journal of Process Control*, 10(5), 487 – 507.

Straus, J. and Skogestad, S. (2017). Economic NMPC for heat-integrated chemical reactors. In *2017 21st International Conference on Process Control (PC)*, 309–314.

Straus, J. and Skogestad, S. (2016). Minimizing the complexity of surrogate models for optimization. In Z. Kravanja and M. Bogataj (eds.), *26th European Symposium on Computer Aided Process Engineering*, volume 38 of *Computer Aided Chemical Engineering*, 289 – 294. Elsevier.

Tan, Y., Moase, W., Manzie, C., Nešić, D., and Mareels, I. (2010). Extremum seeking from 1922 to 2010. In *Proceedings of the 29th Chinese control conference*, 14–26. IEEE.

Wächter, A. and Biegler, L.T. (2006). On the implementation of an interior-point filter line-search algorithm for large-scale nonlinear programming. *Mathematical Programming*, 106(1), 25–57.

Yelchuru, R. and Skogestad, S. (2012). Convex formulations for optimal selection of controlled variables and measurements using mixed integer quadratic programming. *Journal of Process Control*, 22(6), 995 – 1007.