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Economic plantwide control: *Automated controlled variable selection for a reactor-separator-recycle process*

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Abstract: A systematic plantwide control design procedure was proposed in [Skogestad, 2000]. The main goal of this procedure is, to design an optimal control structure for a complete chemical plant based on steady state plant economics, also known as economic plantwide control. In this work, we automated a key step of this procedure, which is the selection of controlled variables, based on quantitative local methods. We applied the economic plantwide control design procedure to a typical chemical plant process, which consists of a reactor, a separator and a recycle stream with purge. We evaluated the economic performance of the designed control structures for various disturbances and found that, although the automatic selection of the controlled variables was based on local methods, the control structures performed quite well, even for large disturbances.

Keywords: Economic plantwide control, Exact local method, Nullspace method, self-optimizing control, control structure selection

1. INTRODUCTION

Production plants today are facing difficult challenges imposed by the modern globalized markets. Global competition demands cheaper and more flexible production, in order to retain profitability and competitiveness. Most of the industrial process control strategies are designed to work at some nominal operating conditions, and usually, are not designed to optimally handle frequent (daily or weekly) changes in market conditions and prices, and thus, to retain an optimal economic operation. Engell [2007] states that, in order to minimize the operation cost, in a such demanding environment of frequent market condition changes, a new look on integration of process control and process operations is needed. In the same paper, Engell provides a review of state of the art in integrated process optimization and control of continuous processes. The two state of the art approaches for implementing an optimal plant operation presented in detail are: the self-optimizing control [Skogestad, 2000] and direct online optimizing control [Marlin and Hrymak, 1997].

For the direct online optimizing control the main idea is, to calculate the optimal input trajectory over some control horizon by optimizing a rigorous nonlinear dynamic model of a plant over some prediction horizon. For self-optimizing control the idea is to turn the optimization into a setpoint control problem and the trick to do that is to find some self-optimizing variables to control. These "magic" variables are defined by Skogestad [2004b] as: the controlled variables, that, when kept constant at nominal optimal values, using the available degrees of freedom, indirectly result in a close-to-optimal operation despite the occurrence of disturbances.

Since the direct online optimization approach guaranties a near-optimal operation, it has gain a lot of attention from process industry, but has failed to be adapted widely by the industry, because it is too complicated and expensive in many cases. Downs and Skogestad [2011] mention that the usual industrial practice is to focus on unit operation control, mainly because this is a simple strategy that is easily understood by the operators and engineers. Thus a plantwide control design procedure has to have three essential characteristics in order to be applied by the process industry engineers: (1) it has to be simple (without the need for complex control technology, like real-time optimization), (2) it has to be able to achieve near-optimal operation, and (3) it should not "require the care and feeding of experts".

The economic plantwide control design procedure, as described in Skogestad [2012], can be used to design control structures that have the first two of the key characteristic mentioned above and the third characteristic could be realized by automating this procedure. The hierarchical decomposition of the economic plantwide control design into a stepwise top-down and bottom up procedures could provide the basic framework for automating the entire design procedure, which is the ulterior goal behind the work presented in this paper. A key step in automating the entire procedure is to automate the selection of the controlled variables for the economic layer. Our main focus here, is to show that this can done by selecting

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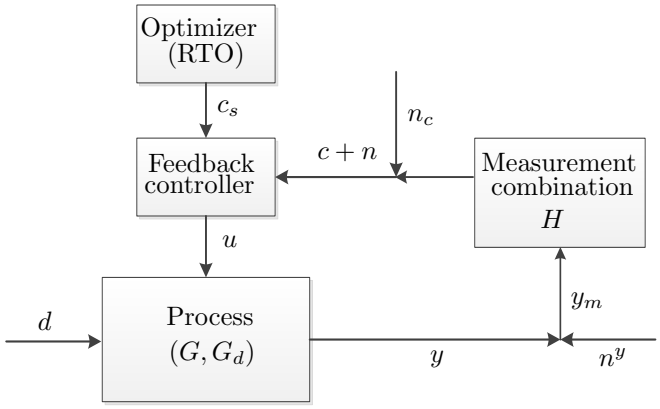


Fig. 1. Feedback implementation of optimal operation with separate layers for optimization (RTO) and control. [Alstad et al., 2009]

self-optimizing controlled variables based the quantitative local methods described in [Alstad et al., 2009].

In this work we apply the economic plantwide control design procedure to a typical chemical plant, emphasizing the automatic selection of the self-optimizing control structure, using quantitative local methods. We evaluate the economic performance of the selected control structures and compare them against a simple strategy of keeping the unused degrees of freedom at their nominal optimal values. As a typical chemical plant, we consider a process, which consists of a reactor, a separator and a recycle stream with purge.

This paper is structured as follows: Section 2 presents a brief summary of the top-down part of the economic plantwide control design procedure. In Section 3, we present a mathematical formulation of optimal operation and the main ideas behind the derivation of Nullspace method and the Exact local method. We describe the reactor-separator-recycle (RSR) process model and the software used for this work in Section 4. A step by step application of the top-down part of the economic plantwide control procedure for the RSR process with emphasis on the automatic selection of self-optimizing CVs is presented in Section 5, and in Section 6 we evaluate the economic performance of these self-optimizing control structures, discuss the results and conclude the paper.

2. ECONOMIC PLANTWIDE CONTROL DESIGN PROCEDURE

This section presents brief summary of the top-down part of the economic plantwide control design procedure as described in Skogestad [2004a] and Skogestad [2012]. The nomenclature for the inputs, disturbances, measurements and noise, used in this section, is depicted in Fig. 1.

Step 1: **Define the operational objectives (economics) and constraints.**

First, operational objectives are defined as a scalar cost function J and the operational constraints are identified and formulated.

Step 2: **Determine the steady-state optimal operation**

In this step, first an operational mode has to be chosen before proceeding with the analysis:

- *Mode 1*: Given throughput (maximize the efficiency). This mode corresponds to some tradeoff between valuable product recovery and minimal energy usage.
- *Mode 2*: Maximum throughput (maximize the production). When the product prices are high compared to energy and raw product prices it is optimal to increase the production to maximum.

(a) **Identify the steady state degrees of freedom**
Identify all the dynamic DOFs $\boldsymbol{u_D}$. They correspond to the actual manipulated variables. Then, exclude all the DOFs, that either don't have any effect on the cost function J or are used to control outputs that have no effect on the cost. The remaining DOFs are the steady state DOFs $\boldsymbol{u_{SS}}$.

(b) **Identify the important disturbances and their expected range**
Here, the important disturbances are identified. The "importance" of a disturbance is proportional to the sensitivity of the cost function to that disturbance. Typically the important disturbances are: the feed flows, feed composition and back-off from constraints.

(c) **Identify the active constraints regions**
Here, the active constraints regions for the expected disturbance range are identified. A straightforward approach, for mapping these regions, is to optimize the process over a fine grid of points in the disturbance space, thus determining which constraints are active at every point. A more resourceful approach, which tracks the active constraint boundaries is reported by Jacobsen and Skogestad [2011].

Step 3: **Select primary (economic) controlled variables.**

Every steady state DOF identified in the step 2(a) needs to be paired with a primary controlled variable.

First, pair them with the active constraints, which can be considered as the obvious self-optimizing variables, since keeping them at the nominal optimal values, results in an optimal operation. The active constraints could be inputs $\boldsymbol{u}$ or outputs $\boldsymbol{y}$. While, the implementation for the active inputs constraints is trivial (e.g. valve fully open or closed), for output constraints that can not be violated, special care, in terms of safety margins (back-off), is required.

Then, select self-optimizing controlled variables for the remaining DOFs . The main steps involving the selection of those variables are:

(a) **Identify the candidate measurements**
Identify all the candidate measurements $\boldsymbol{y}$ and estimate the expected static measurement error $\boldsymbol{n^y}$. The measurements should include the inputs too $\boldsymbol{u}$(e.g. the flow rates measurements).

(b) **Select the primary (economic) controlled variables (CVs) for the remaining DOFs**
As primary CVs $\boldsymbol{c}$ we may select a single or combination of measurements, based on the structure of the $\boldsymbol{H}$ matrix, that is: $\boldsymbol{c = H\,y}$. The selection is based on:

(I) **Qualitative approach** (based on the following Skogestad's heuristic rules)
  (1) The optimal value of a CV should be insensitive to disturbances.
  (2) The CV should be easy to measure and control.
  (3) The CV should be sensitive to manipulated variable (MV) variations.
  (4) For cases with two or more CVs, they should be not closely correlated.

(II) **Quantitative approach**
  (1) **Brute force approach**
    Grid the expected disturbance space and evaluate the cost function J at each point of the grid, including estimated measurement noise, while keeping a subset (of n_u size) of candidate CVs set at their nominal values. Choose for pairing the subset of CVs that gives the lowest cost.
  (2) **Local approaches**
    Local approaches are based on the Taylor series expansion of the cost function around the optimal nominal point. These are: the Maximum gain rule [Skogestad and Postlethwaite, 2005], the Nullspace method and the Exact local method [Alstad et al., 2009].

  The last two local methods are described in the section 3.

Step 4: **Select the location of throughput manipulator (TPM)**

The TPM or the process "gas pedal" is usually a flow in the process that is set. There are two key concerns regarding the location of the TPM:

(a) **Economics**
  The location of the TPM is going to affect how tight some active constraints can be controlled, thus affecting the economic loss.

(b) **Structure of the regulatory control system**
  The location of the TPM has a significant impact on the regulatory control structure, because of the radiation rule [Price and Georgakis, 1993], which links the top-down and the bottom-up parts of this procedure.

We do not consider the bottom-up part of these procedure, because it is out of the scope of this paper. We refer the reader to [Skogestad, 2012].

3. LOCAL QUANTITATIVE METHODS

Here, we focus on step 3(b) of the procedure described in the previous section. We present the mathematical formulation of the optimal operation and the lay down the ideas behind the two local methods, the Nullspace method and the Exact local method. The work presented here is follows [Alstad et al., 2009], unless otherwise stated. The nomenclature used in this section, if not explicitly defined, is depicted in the Fig. 1.

Optimal operation of the plant, with respect to the steady state DOFs $\boldsymbol{u}$, can be defined as:

$$\begin{aligned} \underset{u}{\text{minimize}} \quad & J(\boldsymbol{u},\boldsymbol{d}) \\ \text{subject to} \quad & c_i(\boldsymbol{u},\boldsymbol{d}) \leq 0. \end{aligned} \tag{1}$$

where: the $c_i(\boldsymbol{u},\boldsymbol{d})$ are the operational constraints. We assume that the $\boldsymbol{u}$ here includes only the remaining steady state DOFs and that the $\boldsymbol{d}$ includes the parameter variations too.

For a given $\boldsymbol{d}$, the solution of the problem 1 gives the optimal value for the cost function $J^{opt}(\boldsymbol{d})$, the optimal input values $\boldsymbol{u}^{opt}(\boldsymbol{d})$ and the optimal output values $\boldsymbol{y}^{opt}(\boldsymbol{d})$.

We define the loss as the difference between the cost using non optimal inputs $\boldsymbol{u}$ and the optimal cost $J^{opt}(\boldsymbol{d})$:

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

The linearized (local) model in terms of deviation variables is formulated as:

$$\Delta \boldsymbol{y} = \boldsymbol{G^y}\Delta\boldsymbol{u} + \boldsymbol{G_d^y}\Delta\boldsymbol{d} \tag{3}$$

$$\Delta \boldsymbol{c} = \boldsymbol{H}\boldsymbol{G^y}\Delta\boldsymbol{u} + \boldsymbol{H}\boldsymbol{G_d^y}\Delta\boldsymbol{d} \tag{4}$$

We define the scaled disturbances $\boldsymbol{d'}$ and scaled measurements noise $\boldsymbol{n}^{y'}$ as:

$$\Delta\boldsymbol{d} = \boldsymbol{W_d}\Delta\boldsymbol{d'} \tag{5}$$

$$\boldsymbol{n}^{y} = \boldsymbol{W_{n^y}}\boldsymbol{n}^{y'} \tag{6}$$

The self-optimizing control can be described, in terms of the variables defined in this section, as the selection of optimal $\boldsymbol{H}$ in $\boldsymbol{c} = \boldsymbol{H}\,\boldsymbol{y}$, such that, if $\boldsymbol{c}$ kept at its nominal optimal values $\boldsymbol{c_s}$ (constant set point policy), it results in minimal or acceptable loss [Yelchuru and Skogestad, 2011].

Nullspace method

The derivation of this method is quite straightforward, details can be found in [Alstad et al., 2009]. Assuming that there is no measurement noise $n^y = 0$, an optimal combination of measurements can be formulated as:

$$\Delta\boldsymbol{c}^{opt} = \boldsymbol{H}\Delta\boldsymbol{y}^{opt} \tag{7}$$

$\Delta\boldsymbol{y}^{opt}$ can be written as:

$$\Delta\boldsymbol{y}^{opt} = \boldsymbol{F}\Delta\boldsymbol{d} \tag{8}$$

Combining the equations(7) and (8) results:

$$\Delta\boldsymbol{c}^{opt} = \boldsymbol{H}\boldsymbol{F}\Delta\boldsymbol{d} \tag{9}$$

where: $\boldsymbol{F} = \frac{\partial \boldsymbol{y}^{opt}}{\partial \boldsymbol{d}} = -(\boldsymbol{G^y}\boldsymbol{J_{uu}^{-1}}\boldsymbol{J_{ud}} - \boldsymbol{G_d^y})$ is the optimal sensitivity matrix. For practical purposes its easier to calculate the $\boldsymbol{F}$ by reoptimizing non-linear steady state plant model for small disturbance variations.

An optimal operation based on constant set policy means $\Delta\boldsymbol{c}^{opt} = 0$ for any $\Delta\boldsymbol{d} \neq 0$.

Theorem 1. (Nullspace method). [Alstad et al., 2009] If the number of measurements n_y is equal or larger than the number of inputs n_u plus the number of disturbances n_d, that is $n_y \geq n_u + n_d$ and $\boldsymbol{F}$ is evaluated with constant active constraint set, then it is possible to select the matrix $\boldsymbol{H}$ as a basis for the null space of $\boldsymbol{F}$, $\boldsymbol{H} \in \mathcal{N}(\boldsymbol{F^T})$, such that, $\boldsymbol{HF} = \boldsymbol{0}$

Which means that any $\boldsymbol{H}$ such that, $\boldsymbol{HF} = \boldsymbol{0}$ results in an optimal operation.

Exact local method

To minimize the average and the worst case loss for the expected noise and disturbances, Alstad et al. [2009] formulated the the problem for finding an optimal measurement combination as follows:

$$\boldsymbol{H} = \arg\min_{\boldsymbol{H}} \left\| \boldsymbol{J}_{\boldsymbol{uu}}^{\frac{1}{2}} (\boldsymbol{H}\boldsymbol{G}^{\boldsymbol{y}})^{-1} \boldsymbol{H}\boldsymbol{Y} \right\|_{*} \tag{10}$$

where: $\boldsymbol{Y} = [\boldsymbol{F}\boldsymbol{W}_{\boldsymbol{d}}\, \boldsymbol{W}_{\boldsymbol{n}}]$, the $*$ denotes 2-norm for the worst case scenario and Frobenius norm for minimizing the average loss.

In the same paper the analytical solution for Frobenius norm case of the problem (10) is derived:

$$\boldsymbol{H}^{\boldsymbol{T}} = (\boldsymbol{Y}\boldsymbol{Y}^{\boldsymbol{T}})^{-1}\boldsymbol{G}^{\boldsymbol{y}}(\boldsymbol{G}^{\boldsymbol{y}\boldsymbol{T}}(\boldsymbol{Y}\boldsymbol{Y}^{\boldsymbol{T}})^{-1}\boldsymbol{G}^{\boldsymbol{y}})^{-1}\boldsymbol{J}_{\boldsymbol{uu}}^{\boldsymbol{1/2}} \tag{11}$$

Kariwala et al. [2008] showed that the $\boldsymbol{H}$ obtained for Frobenius norm is in some sense super optimal. It minimizes both worst case loss and the average case loss. Yelchuru and Skogestad [2011] based on the analytical solution (11) derived and proved the following theorem:

Theorem 2. (Simplified analytical solution). [Yelchuru and Skogestad, 2011] Another analytical solution to problem in (10) is

$$\boldsymbol{H}^{\boldsymbol{T}} = (\boldsymbol{Y}\boldsymbol{Y}^{\boldsymbol{T}})^{-1}\boldsymbol{G}^{\boldsymbol{y}}\boldsymbol{Q} \tag{12}$$

where: $\boldsymbol{Q}$ is any non-singular matrix of $n_c \times n_c$

This method is recommended when the measurment noise is not negligible.

4. PROCESS DESCRIPTION

In this section we describe the details of the reactor-separator-recycle process used as a case study in this work.

4.1 Process model description

A model of a generic chemical plant, which consists of a reactor, a separator and a recycle stream with purge, is used as a case study. The specific process was chosen because it incorporates the basic structure of many chemical plants and because it has been studied extensively in the process control literature [Larsson et al., 2003],[Jacobsen and Skogestad, 2011],[Wu and Yu, 1996]. In this work, we used the same process parameters and reaction set as [Jacobsen and Skogestad, 2011], so the reader can refer to that paper for any details omitted here. The process flow diagram is illustrated in Fig. 2.

A fresh feed F_0 of raw product $\mathcal{A}$ and recycle stream R are fed into a continuously stirred tank reactor (CSTR). Two parallel reactions take place in the CSTR:

$$\mathcal{A} \longrightarrow \mathcal{B} \tag{13a}$$
$$\mathcal{A} \longrightarrow 2\,\mathcal{C} \tag{13b}$$

where: $\mathcal{B}$ is the desired product and $\mathcal{C}$ a byproduct. The reaction rates are modelled as first-order kinetics. The reaction rate model is given by:

$$r_i = A_i \exp\left(\frac{E_{\alpha,i}}{\mathcal{R}T}\right) \tag{14}$$

where: $E_{\alpha,i}$ is the activation energy, $\mathcal{R}$ is the gas constant and T is the temperature. The reaction parameters are given in Table 1.

Table 1. Reaction kinetics parameters

Reaction, i	Reaction rate constant, A_i, $[units^{-1}]$	Activation energy, $E_{\alpha,i}$, [J/mol]
$\mathcal{A} \longrightarrow \mathcal{B}$	1×10^5	6×10^4
$\mathcal{A} \longrightarrow 2\,\mathcal{C}$	5×10^6	8×10^4

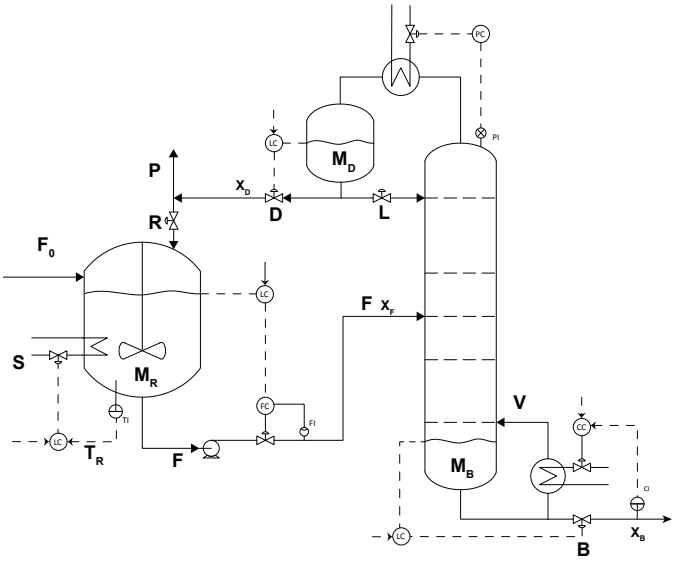


Fig. 2. Process flow diagram for the reactor-separator-recycle process

Table 2. Distillation column parameters

Parameter	Value	Parameter	Value
α_{AC}	0.70	number of stages	30
α_{BC}	0.60	feed stage location	15

The effluent F of the reactor is sent to the distillation column, where the product B is separated as a bottom product and the unreacted A and C are distilled. Part of the distillate D is removed as P purge, while the rest of it R is recycled back to the CSTR.

The column model used here is an ideal multicomponent model based on the "Column A" in [Skogestad and Postlethwaite, 2005]. Some of the column parameters are given in Table 2.

4.2 Process optimization and simulation

For this investigation we developed a steady state MATLAB model and a dynamic SIMULINK model of the described above process. For the optimization needs the builtin MATLAB® non-linear optimization function (**fmincon**) was used. For simulation purposes we used SIMULINK® with ode15s solver.

5. CASE STUDY

This section presents the implementation of the top-down part of the economic plantwide control design procedure as described in [Skogestad, 2004a] and [Skogestad, 2012]. The nomenclature used in this section is depicted in Fig. 2.

Step 1: **Define the operational objectives (economics) and constraints.**

Cost function: The cost function for this process is defined as follows:

$$J = p_F\, F_0 + p_V\, V - p_P\, P - p_B\, B$$

where: F_0 is the reactor feed flow rate, V is the column boilup, B is the bottom product flow rate and P is the purge flow rate. The p_F, p_V, p_B and p_P are their respective prices.

Operational constraints: The operational constraints are the following: the product specifications and equipment limitations.

$$x_{\mathcal{B},B} \leq 0.9 \qquad T_R \leq 390\,[\mathrm{K}]$$
$$M_R \leq 11000\,[\mathrm{mol}] \qquad V \leq 30\,[\mathrm{mol/s}]$$
$$R \geq 0\,[\mathrm{mol/s}] \qquad P \geq 0\,[\mathrm{mol/s}]$$

where: $x_{\mathcal{B},B}$ is the composition of $\mathcal{B}$ in the bottom product stream B, T_R is the reactor temperature, M_R is the reactor holdup, R recycle stream, P purge stream.

Step 2: **Determine the steady-state optimal operation**

For this process we assumed that the feed is given, thus the operational mode is *Mode 1*: Given throughput.

(a) **Identify the optimization degrees of freedom analysis**

Dynamic degrees freedom:

$$\boldsymbol{u_D} = [L, V, D, B, F, R, T_R]$$

Steady state degrees freedom:

$$\boldsymbol{u_{SS}} = [L, V, F, R, T_R]$$

D and B are used to control the levels M_D and M_B respectively, which have no steady state effect on the cost but have to be controlled in order to stabilize the plant.

(b) **Identify the important disturbances and their expected range**

We consider as main disturbance for this case the feed flow, F_0 and the energy price, p_V fluctuations:

$$\boldsymbol{d} = [F_0, p_V]$$

(c) **Identify the active constraints regions**

To map the active constraints regions the disturbance space was gridded into 200×200 points and for each point optimal solution was found. The active constraints regions are illustrated in Fig. 3.

Step 3: **Select primary (economic) controlled variables.**

We assume that the process operates in the first region (I). The nominal operational point is:

$$F_{0,nom} = 0.8\,[\mathrm{kmol/s}], \qquad p_{V,nom} = 0.06\,[\$/\mathrm{mol}]$$

We choose the following pairings (*Input*,*Output*) for the active constraints based on Skogestad's rule [Skogestad, 2012] "pair close".

$$(V, x_{B,B}) \quad (S, T_R) \quad (F, M_R) \quad (R, \text{Closed valve})$$

The control structure of the selected pairings are depicted in Fig 2.

(a) **Identify the candidate measurements**

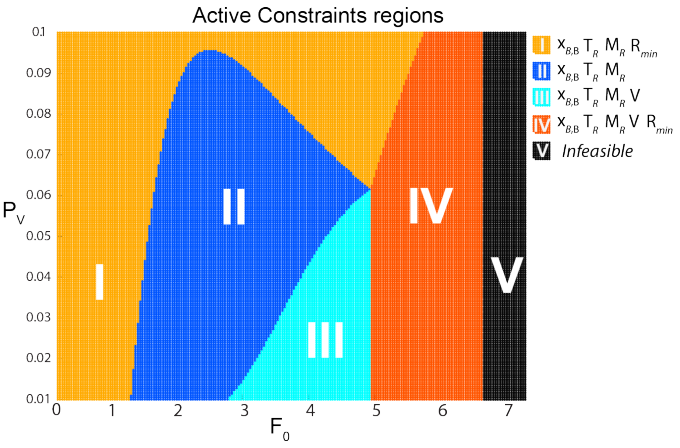


Fig. 3. Active constraints regions for the reactor-separator-recycle process

We assume that the following measurements are available and estimate their expected noise magnitudes:

column and reactor temperatures (*noise* $\pm 1\,[\mathrm{K}]$)
$T_1, T_5, T_9, T_{13}, T_{17}, T_{21}, T_{25}, T_{30}, T_R$,

the input flows (*noise* $\pm 10\,\%$)
L, V, D, B, F, F_0, P

reactor level(*noise* $\pm 100\,[\mathrm{mol}]$)
M_R

compositions (*noise* ± 0.01)
$x_{B,D}, x_{B,B}, x_{B,F}$.

(b) **Select the primary controlled variables for the remaining DOFs**

After pairing the active constraints and levels, only one steady-state DOF is available, and that is the reflux flow, L. We select a self-optimizing controlled variable to pair with L, based on the two quantitative methods, described in section 3 .

First, we calculate the optimal sensitivities $\boldsymbol{F}$ by perturbing the disturbances and re-optimizing the process for the perturbed values:

$$\boldsymbol{F} = \frac{\Delta \boldsymbol{y^{opt}}}{\Delta \boldsymbol{d}}$$

Then, we calculate the gain matrix $\boldsymbol{G^y}$ by perturbing the inputs and then simulating the process until it reaches the new steady state:

$$\boldsymbol{G^y} = \frac{\Delta \boldsymbol{y}}{\Delta \boldsymbol{u}}$$

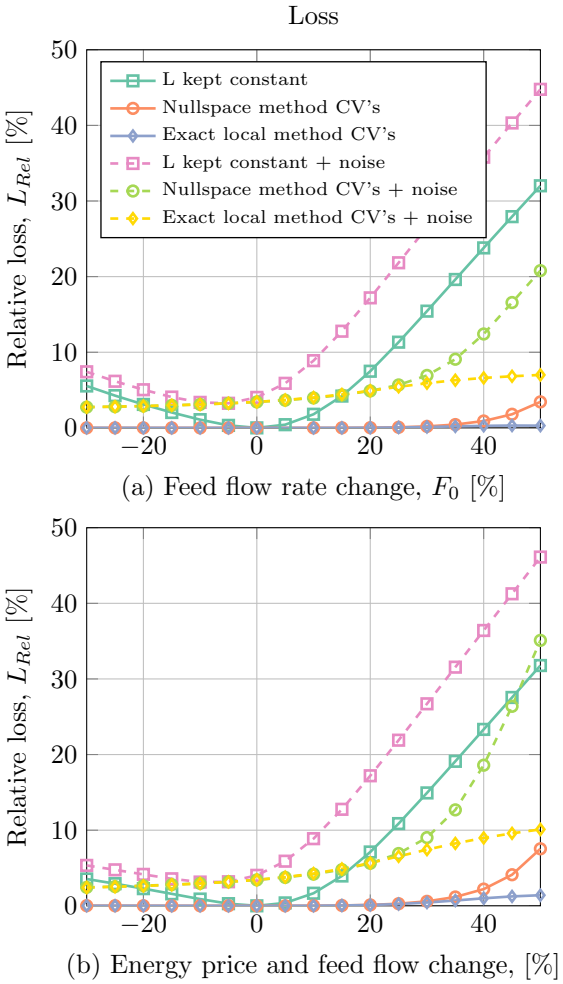
To select an $\boldsymbol{H}$,based on the Nullspace method, we select a basis from the left null space of F^T.

For the selection of $\boldsymbol{H}$ based on the Exact local method we use the equation (12), where we set $\boldsymbol{Q} = \boldsymbol{I}$.

The selection of the self-optimizing control structure for any nominal point has been automated based on the procedure described in this step.

Step 4: **Select the location of throughput manipulator**

For a given feed the TPM is already set by the feed flow F_0. The level control is selected to be in the direction of the flow downstream of the location of the feed. For more details we refer the reader to [Aske and Skogestad, 2009]



(a) Feed flow rate change, F_0 [%]

(b) Energy price and feed flow change, [%]

Fig. 4. Evaluation of the performance of different control structures for various disturbance

6. RESULTS AND CONCLUSIONS

Here we evaluate the economic performance of the self-optimizing control structure against the simplest strategy, that is, to keep the unconstrained degree of freedom L at its nominal optimal value. We disturb the process and evaluate the relative loss L_{Rel} for various disturbances. Where the L_{Rel} is defined as follows:

$$L_{Rel} = \frac{J(\boldsymbol{u}, \boldsymbol{d}) - J^{opt}(\boldsymbol{d})}{J^{opt}(\boldsymbol{d})} \tag{15}$$

The economic performances of all the control structures for different disturbance values are depicted in Fig. 4.

First, we evaluate the relative loss for feed flow changes F_0 for the control structures with and without measurement noise(see Fig. 4(a)). Then, we evaluate the relative loss for simultaneous p_V and F_0 changes for the same control structures (see Fig. 4(b)).

It is clear that keeping the selected self-optimizing controlled variable constant outperforms keeping the L constant in both of the cases. Therefore the systematic selection of the controlled variables based on exact local methods could be considered as a successful approach to automate this essential step of the economic plantwide control procedure

The automation of the economic plantwide design procedure, especially the integration of the automatic design in the major process simulators, could potentially improve the optimality of the production plants on a global scale, thus having a large effect on the production costs and environmental footprint.

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