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 by 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. The interesting and at the same time challenging aspect of the plantwide control design problem, is to design a control structure that ensures stable and close-to-optimal economic operation, and at the same time meets the technical and product quality constraints. These objectives must be satisfied despite the occurrence of disturbances (including market fluctuations, such as: raw material and products price changes, product demand changes, energy price changes, etc.). As Engell and Harjunkoski [2012] stated "the merciless global competition dictates the need for solutions that keep the production cost low and adapt to changing situations".

However, despite the ever-increasing market pressure, the problem of the plantwide control, also known as "control structure design for the complete plant" Skogestad [2004a], is not new. Many different plantwide control design rules have been suggested in the last decades. Larsson and Skogestad [2000] provide an excellent overview of different plantwide control design approaches. As mentioned in Downs and Skogestad [2011], 20 years ago the "Tennessee Eastman Challenge problem" was designed so the various plantwide control design procedures could be tested against each other, but nevertheless, much of the research done during over the previous decades, has *not* gained a significant acceptance by the modern industry.

There are many different plantwide control design approaches, 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. That paper 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 in his paper 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: using rigorous nonlinear steady-state plant model select off-line some "magic" self-optimizing variables. These "magic" variables are defined in 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.

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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. The main idea is to formulate the optimal economic operation as a mathematical optimization problem and then to design a control structure that ensures close-to-optimal operation while satisfying the stability and robustness requirements. The suggested design procedure is split into a top-down part, that aims to finds an optimal control structure based on plant steady state economics, and bottom-up part that aims to find a simple and robust regulatory control structure which can be used under varying economic condition.

The third characteristic could be realized by automating the plantwide control design. An automated procedure could widen the industrial acceptance of state of the art strategies for optimal plant operation, by hiding the unnecessary complexities from the process control engineers, thus having a significant impact on the production costs and environmental footprint on a global scale. 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 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. The specific process flow is selected, because it incorporates the basic structure of most of the 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].

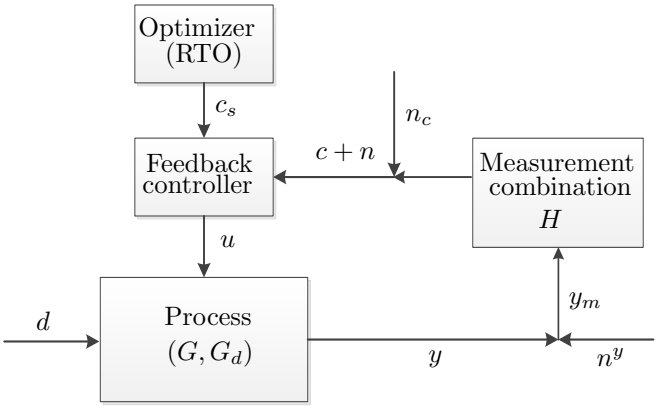

Fig. 1. Feedback implementation of optimal operation with separate layers for optimization (RTO) and control. [Alstad et al., 2009]

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 the 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 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 and discuss the results. Section 7 gives a brief overview the work and concludes 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. For production plants, a typical cost function is:

$$J = \sum p_{F,i} F_{F,i} + \sum p_{U,i} F_{U,i} + \sum p_{P,i} F_{P,i} \quad (1)$$

where: $F_{F,i}$, $F_{U,i}$ and $F_{P,i}$ are the feed, utility and product streams flow rates, respectively. The terms $p_{F,i}$, $p_{U,i}$ and $p_{P,i}$ are their respective prices. Typical operational constraints are: the product quality specifications, process safety requirements, equipment limitations, bounds for temperatures, pressures, flows, etc.

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

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

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- *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 degrees of freedom (DOFs) that affect the cost function J. First, the dynamic DOFs $\boldsymbol{u_D}$ are identified. They correspond to the actual manipulated variables e.g valves and/or other adjustable electrical and mechanical variables. Then, all the DOFs, that either don't have any effect on the cost function J (e.g. an extra bypass valve on a heat exchanger), or are used to control outputs that have no effect on the cost(e.g. valves that are used to control tank levels), are fixed at some realistic value and are excluded from further analysis. The remaining DOFs are the steady state DOFs $\boldsymbol{u_{SS}}$ known also as optimization DOFs.

(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, prices (included in the cost function)and back-off from constraints.

(c) **Identify the active constraints regions**
Here, the active constraints regions for the 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 primarily 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, the self-optimizing controlled variables for the remaining DOFs are identified. 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 loss. While this method is the simplest to understand and apply, it is the most time consuming method. Even if we consider single individual measurements as CV candidates, it still remains almost a hopeless combinatorial optimization problem to attack for large number of inputs n_u and measurements n_y , since it requires $n_{CV_{\text{cmb}}}$ different CV combinations to be considered, where:

$$n_{CV_{\text{cmb}}} = \binom{\boldsymbol{n_y}}{\boldsymbol{n_u}} \tag{2}$$

  (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 [Alstad and Skogestad, 2007] and the Exact local method [Alstad et al., 2009].

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

We note that, Step 3 has to be repeated for each distinct active constraint region. When the process moves to a new region with different active constraints, the control structure must be switched to the one designed for that region. Otherwise this could result a large economic penalty or even infeasibility.

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**

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The location of the TPM has a significant impact on the regulatory control structure, because of the radiation rule [Price and Georgakis, 1993], which states that "a self-consistent the inventory control structure must be radiating around the location of a fixed flow".

The selection of TPM location is a very important step because it links the top-down and the bottom up parts of the procedure.

We do not consider the bottom up 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 2(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:

$$\begin{aligned} \underset{u}{\text{minimize}} \quad & J(\boldsymbol{u}, \boldsymbol{d}) \\ \text{subject to} \quad & c_i(\boldsymbol{u}, \boldsymbol{d}) \leq 0. \end{aligned} \tag{3}$$

where: the $c_i(\boldsymbol{u}, \boldsymbol{d})$ are the operational constraints. We assuming 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 3 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 $J^{opt}(\boldsymbol{d})$:

$$L = J(\boldsymbol{u}, \boldsymbol{d}) - J^{opt}(\boldsymbol{d}) \tag{4}$$

The loss can be approximated around a moving $\boldsymbol{u}^{opt}(\boldsymbol{d})$ using Taylor expansion series. Assuming that the active constraints set doesn't change for a given disturbance, the quadratic approximation of the loss function is derived by Halvorsen et al. [2003]:

$$L = \frac{1}{2}(\boldsymbol{u} - \boldsymbol{u}^{opt})^T \boldsymbol{J_{uu}} (\boldsymbol{u} - \boldsymbol{u}^{opt}) \tag{5}$$

Assuming that the number of independent steady state degrees of freedom $\boldsymbol{u}$ is equal to the independent CVs $\boldsymbol{c}$, that is $n_u = n_c$, the constant set point policy can be formulated as:

$$\Delta \boldsymbol{c} = \boldsymbol{H} \Delta \boldsymbol{y} \tag{6}$$

where: $\Delta \boldsymbol{c} = c - c_s$ denotes the difference between the actual c and the nominal c_s values of CVs. If the noise is included the constant setpoint policy implies that $\boldsymbol{c_s} = \boldsymbol{c} + \boldsymbol{n^y}$

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

$$\Delta \boldsymbol{y} = \boldsymbol{G^y} \Delta \boldsymbol{u} + \boldsymbol{G_d^y} \Delta \boldsymbol{d} \tag{7}$$

$$\Delta \boldsymbol{c} = \boldsymbol{H G^y} \Delta \boldsymbol{u} + \boldsymbol{H G_d^y} \Delta \boldsymbol{d} \tag{8}$$

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

$$\Delta \boldsymbol{d} = \boldsymbol{W_d} \Delta \boldsymbol{d'} \tag{9}$$

$$\boldsymbol{n^y} = \boldsymbol{W_{n^y}} \boldsymbol{n}^{y'} \tag{10}$$

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 and Skogestad, 2007]. Assuming that there is no measurement noise $n^y = 0$, for optimal operation the (6) becomes:

$$\Delta \boldsymbol{c}^{opt} = \boldsymbol{H} \Delta \boldsymbol{y}^{opt} \tag{11}$$

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

$$\Delta \boldsymbol{y}^{opt} = \boldsymbol{F} \Delta \boldsymbol{d} \tag{12}$$

Combining the equations(11) and (12) results:

$$\Delta \boldsymbol{c}^{opt} = \boldsymbol{H F} \Delta \boldsymbol{d} \tag{13}$$

where: $\boldsymbol{F} = \frac{\partial \boldsymbol{y}^{opt}}{\partial \boldsymbol{d}} = -(\boldsymbol{G^y J_{uu}^{-1} J_{ud} - G_d^y})$ 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 and Skogestad, 2007] 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

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

To minimize the average and the worst case loss for the expected noise and disturbances, $\left\| \begin{matrix} \boldsymbol{d} \\ \boldsymbol{n}^{y'} \end{matrix} \right\|_2 \leq 1$ Alstad et al. [2009] formulated the the problem for finding a measurement combination as follows:

$$\boldsymbol{H} = \arg\min_{\boldsymbol{H}} \left\| \boldsymbol{J_{uu}^{\frac{1}{2}} (H G^y)^{-1} H Y} \right\|_* \tag{14}$$

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

In the same paper they derived the analytical solution for Frobenius norm case of the problem (14):

$$\boldsymbol{H^T} = \boldsymbol{(YY^T)^{-1} G^y (G^{yT} (YY^T)^{-1} G^y)^{-1} J_{uu}^{1/2}} \tag{15}$$

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.

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Yelchuru and Skogestad [2011] based on the analytical solution (15) derived and proved the following theorem:

Theorem 2. (Simplified analytical solution). [Yelchuru and Skogestad, 2011] Another analytical solution to problem in (14) is

$$\boldsymbol{H^T = (YY^T)^{-1} G^y Q} \tag{16}$$

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

Which results in a quite elegant solution to the original problem 14.

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 description

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:

$$\mathcal{A} \longrightarrow \mathcal{B} \tag{17a}$$
$$\mathcal{A} \longrightarrow 2\,\mathcal{C} \tag{17b}$$

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:

$$r_i = A_i \exp\left(\frac{E_{\alpha,i}}{\mathcal{R}T}\right) \tag{18}$$

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.

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 distilate D is removed as P purge, while the rest of it R is recycled back to the CSTR.

The column model used here is a ideal multicomponent model based on the "Column A" in [Skogestad and Postlethwaite, 2005]. The main assumptions in the model are: constant relative volatilities, constant molar overflows, constant pressure over the column, liquid dynamics based on Francis' wier equation. Some of the column parameters are given in Table 2. The column tray temperatures are estmated using:

$$T_j = \sum x_{i,j}\, T_{b,i} \tag{19}$$

where: T_j is the temperature of the j_{th} tray, $T_{b,i}$ is the boiling temperature of the pure component i and $x_{i,j}$ is the composition of component i in the j_{th} tray.

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

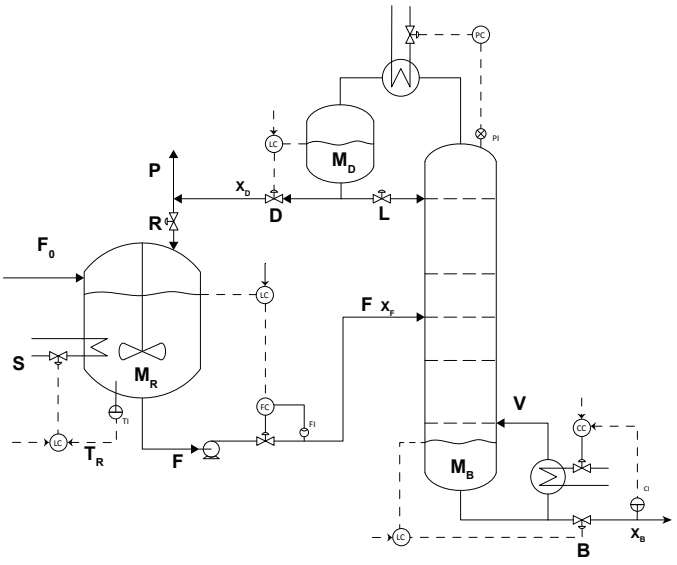

Fig. 2. Process flow diagram for the reactor-separator-recycle process

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

Table 3. Nominal process values

Parameter	Value
$[T_{b,A}, T_{b,B}, T_{b,C}]$	[370, 400, 340] [K]
$[p_V, p_B, p_F, p_P]$	[0.01, 2, 1, 0.5] [$/mol]
F_0	0.8 [kmol/s]

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. ECONOMIC PLANTWIDE CONTROL DESIGN IMPLEMENTATION

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 is derived based on (1):

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

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 constrants: For this process the operational constraints are: the product specification and equipment limitations.

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

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 for stabilizing the plant.

(b) **Identify the important disturbances and their expected range**
We consider as main disturbances for this case the energy price, p_V and the feed flow, F_0 :

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

(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. There are four distinct regions, where various constraints are active and a fifth region of operational infeasibility, where there is no longer possible to handle more feed without violating some of the constraints:

(**I**) $x_{B,B}, T_R, M_R, R$
(**II**) $x_{B,B}, T_R, M_R$
(**III**) $x_{B,B}, T_R, M_R, V$
(**IV**) $x_{B,B}, T_R, M_R, V, R$
(**V**) **Infeasible**

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

We assume nominally 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 pairings (*Input,Output*) as follows: for the the output constraints based on Skogestad's rule "pair close"[Skogestad, 2012] and for the inputs we just fully open or close them.

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

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

(a) **Identify the candidate measurements**
We select the following measurements and estimate the expected noise magnitudes:
column and reactor temperatures (*noise* ± 1 [K])
$T_1, T_5, T_9, T_{13}, T_{17}, T_{21}, T_{25}, T_{30}, T_R$,
the input flows (*noise* $\pm 2\,\%$)
L, V, D, B, F, F_0, P
reactor level(*noise* ± 100 [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 1 DOF left , that is L. Based on the two qualitative methods, described in 3 we select a self-optimizing controlled variable to pair it with L.
First, we calculate the optimal sensitivities $\boldsymbol{F}$ by perturbing the disturbances and re-optimizing the process for the perturbed values. The optimal deviations of the measurements divided by the variation of disturbances provide the $\boldsymbol{F}$ matrix:

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

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. The gain matrix is calculated by dividing the measurements variations by the input deviation:

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

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 (16), 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. We use the steady state process model in MATLAB for the optimization part and dynamic model in SIMULINK for the simulations.
We evaluate the performance of these control structures against keeping the L at its nominal optimal value, in the section 6.

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]

6. EVALUATION OF LOSS BASED ON DYNAMIC PLANT SIMULATIONS

Here we evaluate the economic performance of the self-optimizing control structures (CV's selected based on the Nullspace method and the Exact local method) against the simplest strategy, that is, to keep the unconstrained degree

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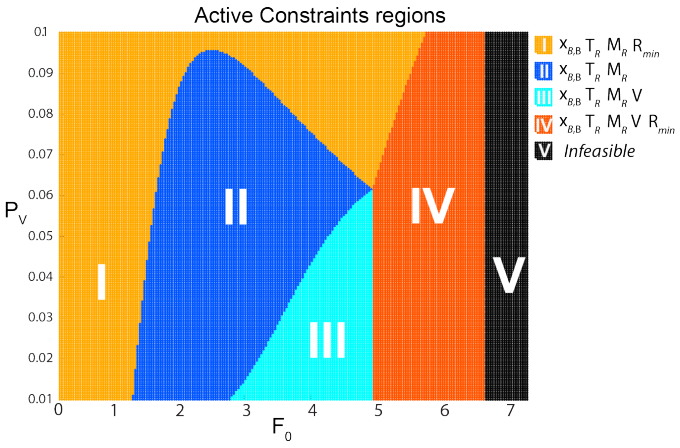


Fig. 3. Active constraints regions for the reactor-separator-recycle process

of freedom L at its nominal optimal value. We disturb the process and evaluate the loss for various disturbances. The economic performance for different disturbance values is depicted in Fig. 6.

First, we evaluate the loss for feed flow changes F_0 for the control structures with and without measurement noise(see Fig. 6(a)). Then, we evaluate the loss for the energy price changes p_V. Again this is done for all the control structures with and without noise (see Fig. 6(b)). Last, we evaluate the loss for simultaneous p_V and F_0 changes for the same control structures (see Fig. 6(c)).

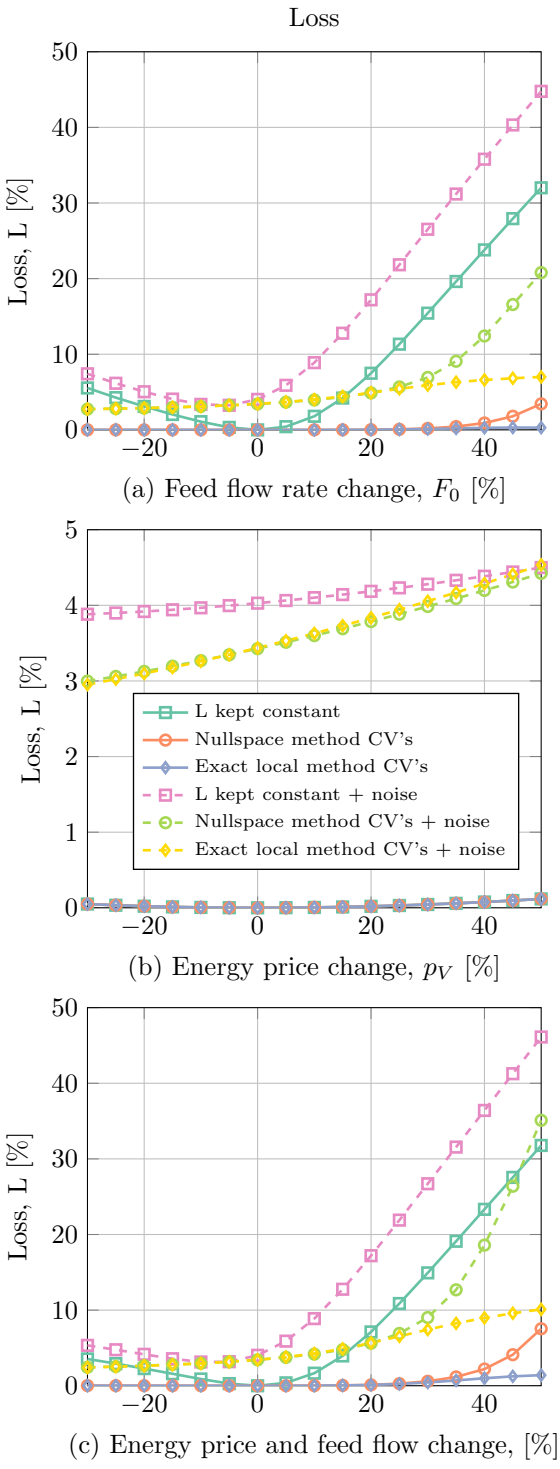
We can clearly see that the self-optimizing control structures outperforms the simple strategy for the feed flow changes case and the simultaneous energy price and feed flow changes case, as shown in Fig. 6(a)) and Fig. 6(c)) respectively. For the case with only energy price changes the performance is simular all for the control structures, as can be seen in Fig. 6(b)). This maybe explained by the high sensitivity of the cost function to changes in feed flow $F0$ and low sensitive to changes in energy price p_V for this nominal operational point.

As can bee seen in all the subfigures of Fig. 6, the performance of the Nullspace based control structure is very simular to the one based on Exact local based for cases with noise, despite the fact that the Nullspace method doesn't take account the noise. This may be explained by relatively low sensitivity of the cost function to noise, thus making the noise negligible.

7. DISCUSSION AND CONCLUSION

We introduced this work by identifying the demand for optimal and more flexible production, imposed by the modern globalized competition. In order to minimize the operation cost in an environment of frequent market condition changes, an integrated process control and optimization approach is needed [Engell, 2007].

We presented briefly two state of the art integrated approaches: the self-optimizing control and direct online optimization control, and argued that, in order for a control structure design procedure to be widely accepted by the process control industry it to has be [Downs and Skogestad, 2011]: (1) simple, (2) efficient (resulting in an optimal operation), (3) should not require a very high expertise.



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

(b) Energy price change, p_V [%]

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

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

We identified that the economic plantwide control design procedure can be used to design control structures that fulfil the (2) and (3) requirements. But in order to fulfil the requirement (1), we could simplify the control structure design procedure, by automating it, thus hiding the unnecessary complexities.

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The hierarchical decomposition of the economic plantwide control to stepwise top-down and bottom-up parts could provides a solid framework for automating the entire design procedure, which is the ulterior goal behind this work.

We identified, as a key step to automate the entire procedure, the automatization of the controlled variables selection for the economic layer. In this work, we show that this can be done quite efficiently based on the quantitative local methods, described in [Alstad et al., 2009].

We present the main algorithm for the economic plantwide control design procedure, emphasizing the systematic selection of the self-optimizing control structure, using quantitative local methods. To understand better these methods we present a mathimatical formulation of the optimal economic operation and lay the basis for the derivation of the two local methods: the Nullspace method and the Exact local method. We present briefly the use of these methods to select the self-optimizing controlled variables.

As a case study, we apply the economic plantwide control design procedure to a process, which consists of a reactor, a separator and a recycle stream with purge. The specific process flow is selected because it incorporates the basic structure of most of the 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]

We evaluate the economic performance of the designed control structures, and compare them against a simple strategy of keeping the unused degrees of freedom at their nominal optimal values. We found that, although the automatic selection of the self-optimizing controlled variables was based on local methods, they performed quite well even for large disturbances. Therefore the systematic selection of the controlled variables based on quantitative local basis 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.

REFERENCES

Vidar Alstad and Sigurd Skogestad. Null Space Method for Selecting Optimal Measurement Combinations as Controlled Variables. *Industrial & Engineering Chemistry Research*, 46(3):846–853, January 2007. ISSN 0888-5885.

Vidar Alstad, Sigurd Skogestad, and Eduardo S. Hori. Optimal measurement combinations as controlled variables. *Journal of Process Control*, 19(1):138–148, January 2009. ISSN 09591524.

Elvira Marie B. Aske and Sigurd Skogestad. Consistent Inventory Control. *Industrial & Engineering Chemistry Research*, 48(24):10892–10902, December 2009. ISSN 0888-5885.

James J. Downs and Sigurd Skogestad. An industrial and academic perspective on plantwide control. *Annual Reviews in Control*, 35(1):99–110, April 2011. ISSN 13675788.

Sebastian Engell. Feedback control for optimal process operation. *Journal of Process Control*, 17(3):203–219, March 2007. ISSN 09591524.

Sebastian Engell and Iiro Harjunkoski. Optimal operation: Scheduling, advanced control and their integration. *Computers & Chemical Engineering*, 47(null):121–133, December 2012. ISSN 00981354.

Ivar J. Halvorsen, Sigurd Skogestad, John C. Morud, and Vidar Alstad. Optimal Selection of Controlled Variables . *Industrial & Engineering Chemistry Research*, July 2003. ISSN 0888-5885.

Magnus G. Jacobsen and Sigurd Skogestad. Active Constraint Regions for Optimal Operation of Chemical Processes. *Industrial & Engineering Chemistry Research*, 50 (19):11226–11236, October 2011. ISSN 0888-5885.

Vinay Kariwala, Yi Cao, and S. Janardhanan. Local Self-Optimizing Control with Average Loss Minimization. *Industrial & Engineering Chemistry Research*, 47(4): 1150–1158, February 2008. ISSN 0888-5885.

T. Larsson, M. S. Govatsmark, S. Skogestad, and C. C. Yu. Control Structure Selection for Reactor, Separator, and Recycle Processes. *Industrial & Engineering Chemistry Research*, March 2003. ISSN 0888-5885.

Truls Larsson and Sigurd Skogestad. Plantwide control - A review and a new design procedure. *Modeling, Identification and Control: A Norwegian Research Bulletin*, 21(4):209–240, January 2000. ISSN 0332-7353.

T E Marlin and A N Hrymak. Real-time operations optimization of continuous processes. *CPC*, 1997.

Randel M. Price and Christos Georgakis. Plantwide regulatory control design procedure using a tiered framework. *Industrial & Engineering Chemistry Research*, 32 (11):2693–2705, November 1993. ISSN 0888-5885.

Sigurd Skogestad. Plantwide control: the search for the self-optimizing control structure. *Journal of Process Control*, October 2000. ISSN 09591524.

Sigurd Skogestad. Control structure design for complete chemical plants. *Computers & Chemical Engineering*, January 2004a. ISSN 00981354.

Sigurd Skogestad. Near-optimal operation by self-optimizing control: from process control to marathon running and business systems. *Computers & Chemical Engineering*, December 2004b. ISSN 00981354.

Sigurd Skogestad. Economic Plantwide Control. In *Plantwide Control*, pages 229–251. John Wiley & Sons, Ltd, 2012.

Sigurd Skogestad and Ian Postlethwaite. *Multivariable Feedback Control: Analysis and Design*. Wiley-Interscience, 2005. ISBN 0470011688.

Kwo-Liang Wu and Cheng-Ching Yu. Reactor/separator processes with recycle1. Candidate control structure for operability. *Computers & Chemical Engineering*, 20 (11):1291–1316, January 1996. ISSN 00981354.

Ramprasad Yelchuru and Sigurd Skogestad. Optimal Controlled Variable Selection with Structural Constraints Using MIQP Formulations? In *IFAC Congress, Milano, Italy*, 2011.

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