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Self-Optimizing Steady-State Back-Off Approach for Control Structure Selection

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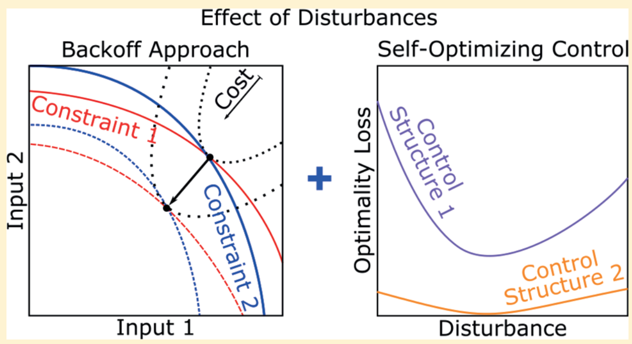
ABSTRACT: The selection of suitable control structures has an important influence on the economic performance of process systems in the presence of disturbances. Economics has been incorporated in the control structure selection problem using different formulations based on different criteria. The back-off approach is based on the idea of minimizing the economic loss that results from the need to back off from the active constraints to avoid violating them in the presence of disturbances. On the other hand, self-optimizing control schemes aim at selecting controlled variables and constant setpoint values, such that the economic loss with respect to optimal operation is minimized in the presence of disturbances. This paper presents a comprehensive study of different formulations of the back-off approach that pays attention to steady-state feasibility in the presence of disturbances. We argue that the back-off approach that selects controlled variables and optimal setpoint values by minimizing the average cost in the presence of disturbances is a global self-optimizing control approach. The performance of the different formulations is compared by means of three different case studies.



1. INTRODUCTION

Control structure (CS) selection involves the selection of controlled variables (CVs), manipulated variables (MVs), the control policy (decentralized or centralized), the controller technology (classical or advanced), the pairing between the CVs and the MVs in the case of a decentralized controller, and the tuning of the controllers. Historically, the design of a plantwide control system has been based on heuristics, mathematical understanding, and process knowledge.[1−3]

This paper considers the problem of control structure selection based on economics in the presence of disturbances and constraints. This problem has been studied by many researchers in the last 35 years using different criteria for incorporating economics in the control structure selection problem or for combining economic objectives with other objectives such as stability and controllability and using different simplifications and approximations to formulate the control structure selection problem. There is also a vast literature wherein the control structure selection problem has been integrated with the design problem.[4−6] Because the dynamic performance of a process strongly depends on its design, and due to conflicts between economy and controllability of chemical processes, there are strong incentives for integrating plant design and control structure decisions.[6] Two strategies for control structure selection based on economics that have been studied independently by different researchers are the back-off approach and self-optimizing control.

1.1. Back-Off Approach. The optimal operating point of an industrial plant is often located at the intersection of the active constraints. However, in the presence of disturbances it is necessary to back off from the constraint boundaries to avoid constraint violations. The size of the back-offs depends on the variability of the constrained variables for the closed-loop controlled system. Many back-off approaches found in the literature have been formulated for the integration of process design and control. By fixing the variables that define the design and topology of the open-loop plant, these formulations reduce to a control structure selection problem. The back-off approach for process control structure selection is based on the idea of selecting the control structure that minimizes the economic cost associated with the required constraint back-offs. A list of back-off approaches found in the literature is provided in Table 1.

Several classifications are possible for back-off approaches:

- Steady-State Economics vs Dynamic Economics: A general framework consists in formulating the control structure selection problem as a mixed-integer dynamic optimization (MIDO) problem, wherein the dynamic economics of the controlled plant are optimized for a

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Table 1. Representative Literature on the Back-off Approach

	steady-state economics	dynamic economics	nominal cost	average cost	steady-state back-off	dynamic back-off	back-off problem	CS selection problem
Bahri et al.[7]	√		√		√		√	
Bahri et al.[8]	√		√			√	√	
Figueroa et al.[9]	√		√			√	√	
Narraway et al.[10]	√		√			√	√	
Loeblein and Perkins[11]	√		√			√	√	
Soliman et al.[12]	√		√			√	√	
Narraway and Perkins[13]	√		√			√		√
Heath et al.[14]	√		√			√		√
Psaltis et al.[15]	√		√			√		√
Zumoffen et al.[16]	√		√			√		√
Kookos and Perkins[17]	√		√			√		√
Kookos and Perkins[18]	√		√		√			√
Kookos and Perkins[18]	√		√			√	√	
Kookos and Perkins[19]	√		√			√		√
Kookos[20]	√			√	√			√
Sharifzadeh and Thornhill[21]	√			√	√			√
Sharifzadeh and Thornhill[22]	√			√		√		√
Mohideen et al.[23]		√		√		√		√
Bansal et al.[24]		√		√		√		√
Sakizlis et al.[25]		√		√		√		√
Yuan et al.[5]		√		√		√		√

given time period[23−25] (see also Yuan et al.[5] and references therein). In these approaches, the disturbance dynamics are specified a priori. However, because continuously operating plants are typically designed to operate at steady-state conditions, many back-off approaches evaluate the economics of operation at steady state.[7−22]

- Nominal Cost vs Average Cost: The evaluation of economic performance has been incorporated using different criteria. Several back-off approaches proceed by minimizing the nominal cost.[7−19] The cost is evaluated only for the nominal values of the disturbances, while the variations of the disturbances with respect to their nominal values are used to evaluate the back-offs. Another criterion is to minimize the expected cost, which can be approximated as a weighted average over a specified (or sampled) set of disturbance scenarios.[20−25]
- Steady-State Back-Offs vs Dynamic Back-Offs: Steady-state back-off approaches are only concerned with avoiding constraint violations at steady state. The back-offs are determined by computing optimal setpoint values such that steady-state feasibility is guaranteed for all disturbance scenarios.[18,20,21] These approaches use a steady-state model of the process and do not require modeling the controller or defining the controller technology and tuning its parameters. The only assumption is that the controllers have integral action, i.e., the controlled variables match their setpoint values at steady state. On the other hand, dynamic back-off approaches pay attention to constraint violations during transient operation (even if the economic cost might be evaluated at steady state).[8−17,19,22−25] These approaches require modeling the dynamic behavior of the closed-loop plant in the presence of disturbances. For each control structure, the set of differential and algebraic equations of the controllers need to be synthesized analytically. The controller's parameters may be either optimized or tuned automatically using analytical rules. To avoid the complexities posed by modeling the controllers, the assumption of perfect control has often been made.[13−15,17,22] While this assumption might be useful for selecting the control structure, it leads to dynamic back-offs equal to zero for the controlled variables, which may lead to constraint violations in practice. Hence, when perfect control is assumed, the back-offs for the selected control structure need to be reevaluated by means of dynamic simulations after modeling the controllers.
- Back-Off Problem vs Control Structure Selection Problem: The back-off problem is typically formulated as a nonlinear programming (NLP) problem, which is solved for a given (fixed) control structure.[8−12] The problem may consist of finding optimal setpoint values that pay attention to constraint feasibility for a given set of disturbance scenarios, or in directly computing the back-offs with respect to the nominal optimal operation and then evaluating the associated economic loss. Based on the back-off approach, the control structure selection problem incorporates binary variables that are used to determine the optimal control structure.[13−25] The problem may be formulated as a MIDO or a mixed-integer nonlinear programming (MINLP) problem. Several simplifications and approximations have been proposed for reducing the computational load of the problem (for example, linearizing the steady-state and dynamic model equations and approximating the problem as a mixed-integer linear programming (MILP) problem[13−15] and including the perfect control assumption).[13−15,17,22]

1.2. Self-Optimizing Control. Self-optimizing control (SOC) aims at selecting controlled variables and constant setpoint values such that, in the presence of disturbances, the closed-loop plant reaches a steady state operating point with an

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acceptable economic loss.[26−28] Most of the SOC approaches found in the literature are local methods.[28] Most local SOC methods are based on the assumption that the set of active constraints does not change with the disturbance values. With this assumption, it is optimal (from a steady-state perspective) to control the active input and output variables at their optimal boundary values, which requires assigning a number of input variables to control these active constraints. This permits us to view the optimization problem as an unconstrained problem in the reduced input space that is left after satisfying all the active constraints. Local SOC methods aim at selecting additional controlled variables such that these remaining inputs reach near-optimal values at steady state when disturbances occur. A particularity of most SOC approaches is that these additional controlled variables are selected as linear combinations of the output and input variables.

Based on the first-order variation of the necessary conditions of optimality (NCO) for an unconstrained optimization problem and a linearized model of the output variables, Halvorsen et al.[27] derived a local expression for the economic loss as a function of the disturbance values and the measurement error. This local loss expression was used to derive optimal linear combinations of measurements that minimize the (local) worst-case loss[27] and the (local) average loss[29] in the presence of disturbances. Another local SOC method is the null space method proposed by Alstad and Skogestad,[30] which consists in selecting as controlled variables linear combinations of measurements that lie in the null space of the sensitivity matrix of the optimal outputs with respect to the disturbances. Later on, Alstad et al.[31] showed that (in the absence of implementation error) the null space method zeroes the local loss expression derived by Halvorsen et al.[27] The equivalence between the null space method and gradient control has been established[32] as well as its equivalence with neighboring-extremal control.[33] A formulation of the null space method in the whole input space is presented in Marchetti and Zumoffen[34] for constrained problems with active constraints. In local SOC methods,[29−31,34] the setpoint values for the linear combinations of measurements are selected as the values of these linear combinations evaluated at the nominal optimum.

Because, in many practical applications, the set of active constraints does change with the disturbance values, variants of the local SOC methods have been proposed to handle changes in the active set. For instance, Manum and Skogestad[35] use a parametric programming approach to determine the active set regions and proposed the selection of the controlled variables by applying the null space method within each region. The values of the controlled variables for each region are used to decide when to switch regions. Instead of detecting the active set and changing the control structure, Hu et al.[36] proposed a local approach for finding a single control structure that guarantees feasibility for all disturbance values within pre-specified bounds. The optimal linear combination control structure is obtained by minimizing the average local loss subject to linearized constraints.

Recently, Ye et al.[37] proposed a global SOC approach that is restricted to problems for which the set of active constraints is invariant. Instead of relying on the local loss computed at the nominal optimum only, a number of disturbance scenarios is randomly sampled, and the optimization problem is solved for each scenario. For each disturbance scenario, the corresponding local loss expression is computed, and the optimal linear combination of measurements, together with their corresponding optimal setpoint values, are found by minimizing the average loss. A variant of this approach, which also uses local information for each disturbance scenario, was extended to constrained problems with active set changes.[38] Notice that the difference between local and global SOC methods is that local SOC methods rely on optimality information obtained at a single optimal operating point, which corresponds to the nominal disturbance values (the nominal optimum), whereas global SOC methods rely on optimality information obtained for a representative (e.g., sampled) set of disturbance scenarios. A review of local and global SOC approaches can be found in Jäschke et al.[28]

1.3. Contributions of This Work. The focus of this paper is on steady-state back-off approaches. Hence, we are concerned with avoiding constraint violations only at steady-state operation in the presence of disturbances. We present a comparative study analyzing the difference between minimizing the nominal cost and the average cost. We notice that the steady-state back-off approach and self-optimizing control share the same objectives, and we argue that the back-off approach with average cost minimization represents a global SOC problem. The contributions of this work are the following:

- By means of simple tutorial case studies, we present a comparative study between the steady-state back-off approach with nominal cost minimization and average cost minimization.
- Because, for the purpose of control structure selection, minimizing the average cost is equivalent to minimizing the average loss, we argue that the steady-state back-off problem with average cost minimization is a global SOC approach. This is verified by means of a comparative study concerning the operation of a CSTR reactor, where the performance of the approach is compared to that of a local SOC method, such as the null space method.
- We consider two different formulations of the steady-state back-off problem with average cost minimization. The first formulation consists in an MINLP that selects the best classical control structure, while the second formulation is an NLP that selects optimal linear combinations of input and output variables as controlled variables. Both formulations are global SOC approaches that find optimal setpoint values for the controlled variables and for the fixed inputs that are not used as manipulated variables while guaranteeing constraint satisfaction for a set of disturbance scenarios. The MINLP formulation is very similar to the formulation for control structure selection based on economics proposed by Kookos.[20]
- We include in the MINLP formulation additional linear constraints that are used to bound the elements of the RGA matrix of the selected control structure. We show that these additional constraints may help avoid obtaining an unsuitable control structure.
- We present two alternative convex mixed integer quadratic programming (MIQP) approximations of the MINLP formulation. The first MIQP approximation is local in the inputs and global in the disturbances, while the second MIQP is local in both the inputs and disturbances.
- In three case studies, we compare the performance obtained by the best classical control structure with the performance of an optimal linear combination control structure. It is shown that by controlling appropriate

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linear combinations of input and output variables, it might be possible to improve the economic performance of the controlled plant at steady state. While in the SOC literature, the selection of linear combination control structures has been aimed at achieving near-optimal conditions for the unconstrained degrees of freedom, in our first case study, we show that they are also useful in cases in which the optimum is completely determined by the intersection of active constraints, and the set of active constraints changes with the disturbance values.

- Based on our study, we provide a number of recommendations for steady-state back-off approaches and SOC.

The paper is organized as follows. Preliminary material is presented in section 2, including the formulation of the optimization problem, the steady-state back-off approach and self-optimizing control. Two different steady-state back-off formulations with average cost minimization are presented in section 3: (i) an MINLP problem that selects the optimal classical CS and (ii) an NLP problem that selects optimal linear combinations of output and input variables as controlled variables. Section 4 presents two alternative MIQP approximations of the MINLP problem. The different CS selection strategies are applied to three different case studies in section 5. Finally, section 6 concludes the paper and presents a number of recommendations.

2. PRELIMINARIES

2.1. Problem Formulation. The open-loop behavior of the plant can be represented by the following system of differential algebraic equations:

$$\mathbf{f_D}(\dot{\mathbf{x}}, \mathbf{x}, \mathbf{w}, \mathbf{u}, \mathbf{d}) = \mathbf{0} \tag{1a}$$

$$\mathbf{f_A}(\mathbf{x}, \mathbf{w}, \mathbf{u}, \mathbf{d}) = \mathbf{0} \tag{1b}$$

$$\mathbf{y} = \mathbf{F}(\mathbf{x}, \mathbf{w}, \mathbf{u}, \mathbf{d}) \tag{1c}$$

where $\mathbf{x} \in \mathbb{R}^{n_x}$ is the vector of state variables, $\mathbf{w} \in \mathbb{R}^{n_w}$ is the vector of algebraic variables, $\mathbf{u} \in \mathbb{R}^{n_u}$ is the vector of input (decision) variables, $\mathbf{d} \in \mathbb{R}^{n_d}$ is the vector of uncertain parameters and disturbances, $\mathbf{f_D}$ is the vector of n_x differential equations, $\mathbf{f_A}$ is the vector of n_w algebraic equations, and $\mathbf{y} \in \mathbb{R}^{n_y}$ is the vector of measured output variables.

Continuously operating plants are typically designed to operate at steady-state conditions. The optimum steady-state operating point is given by the solution of the following NLP problem:

$$\min_{\mathbf{x},\mathbf{w},\mathbf{u}} J(\mathbf{x}, \mathbf{w}, \mathbf{u}, \mathbf{d}) \tag{2a}$$

$$\text{s.t. } \mathbf{f_D}(\mathbf{0}, \mathbf{x}, \mathbf{w}, \mathbf{u}, \mathbf{d}) = \mathbf{0} \tag{2b}$$

$$\mathbf{f_A}(\mathbf{x}, \mathbf{w}, \mathbf{u}, \mathbf{d}) = \mathbf{0} \tag{2c}$$

$$\mathbf{y}^{\mathrm{L}} \leq \mathbf{y} = \mathbf{F}(\mathbf{x}, \mathbf{w}, \mathbf{u}, \mathbf{d}) \leq \mathbf{y}^{\mathrm{U}} \tag{2d}$$

$$\mathbf{u}^{\mathrm{L}} \leq \mathbf{u} \leq \mathbf{u}^{\mathrm{U}} \tag{2e}$$

where J is the economic objective function (or cost) to be minimized, $\mathbf{y}^{\mathrm{L}}$ and $\mathbf{y}^{\mathrm{U}}$ are the lower and upper bounds on the output variables, while $\mathbf{u}^{\mathrm{L}}$ and $\mathbf{u}^{\mathrm{U}}$ are the lower and upper bounds on the input variables.

Let us introduce the input−output mappings $\mathbf{y}(\mathbf{u},\mathbf{d})$ and $J(\mathbf{u},\mathbf{d})$, which correspond to the steady-state behavior of the process. Note that the evaluation of these mappings requires solving the system (2b and 2c) for $\mathbf{x}$ and $\mathbf{w}$ for given values of $\mathbf{u}$ and $\mathbf{d}$ and then evaluating $\mathbf{y}$ from (1c) and J from (2a). By using these mappings, Problem (2) can be written in a compact form as follows:

$$\min_{\mathbf{u}} J(\mathbf{u}, \mathbf{d}) \tag{3a}$$

$$\text{s.t. } \mathbf{y}^{\mathrm{L}} \leq \mathbf{y}(\mathbf{u}, \mathbf{d}) \leq \mathbf{y}^{\mathrm{U}} \tag{3b}$$

$$\mathbf{u}^{\mathrm{L}} \leq \mathbf{u} \leq \mathbf{u}^{\mathrm{U}} \tag{3c}$$

Problem (3) is defined for a given value of the disturbance vector $\mathbf{d}$. We denote by $\mathbf{u}^*(\mathbf{d})$ the optimal input of Problem (3) as a function of the disturbance values. Note that the set of active constraints may change for different values of $\mathbf{d}$.

The nominal disturbance values, denoted as $\mathbf{d}_{\mathrm{n}}$, represent the best known or average values for each disturbance. In this paper, we assume the disturbances belong to a disturbance set $\mathcal{D}$ containing all possible realizations of the disturbances. The set $\mathcal{D}$ is typically defined by considering box constraints of the form $\mathcal{D} = \{\mathbf{d} \in \mathbb{R}^{n_d}\text{: } \mathbf{d}^{\mathrm{L}} \leq \mathbf{d} \leq \mathbf{d}^{\mathrm{U}}\}$.

2.2. Steady-State Back-Off Approach with Nominal Cost Minimization. The aim of the steady-state back-off problem is to determine the control structure and the setpoint values that minimize the cost for the nominal disturbance values while guaranteeing steady-state feasibility for all possible disturbances $\mathbf{d} \in \mathcal{D}$. Let $\mathbf{z}$ denote the vector of binary variables that determines the choice of the control structure. For a given $\mathbf{z}$, it is possible to construct the vector $\mathbf{r}(\mathbf{z}, \mathbf{u}, \mathbf{y}) \in \mathbb{R}^{n_u}$, which includes the selected controlled output variables and the fixed input variables. The input variables that are not included in $\mathbf{r}(\mathbf{z},\mathbf{u},\mathbf{y})$ are the selected manipulated variables. Likewise, we introduce the vector $\mathbf{r}^{\mathrm{sp}} \in \mathbb{R}^{n_u}$, which includes the setpoint values for the controlled output variables and the target values for the fixed inputs. This way, the effect of the controller on the steady-state behavior of the controlled plant can be accounted for by introducing the following n_{u} equations:

$$\mathbf{r}(\mathbf{z}, \mathbf{u}, \mathbf{y}(\mathbf{u}, \mathbf{d})) = \mathbf{r}^{\mathrm{sp}} \tag{4}$$

Here, we assume that the controller is designed with integral action and that the manipulated variables $\mathbf{u}$ reached by the controlled plant at steady state can be computed by solving (4) for $\mathbf{d}$ and $\mathbf{r}^{\mathrm{sp}}$ given. The closed-loop steady-state back-off problem can now be formulated as follows:

$$\begin{aligned} &\min_{\mathbf{z},\mathbf{r}^{\mathrm{sp}}} J(\mathbf{u}_n, \mathbf{d}_n) \\ &\text{s.t. } \mathbf{r}(\mathbf{z}, \mathbf{u}_n, \mathbf{y}(\mathbf{u}_n, \mathbf{d}_n)) = \mathbf{r}^{\mathrm{sp}}, \quad \mathbf{d}_n \in \mathcal{D} \\ &\quad \mathbf{r}(\mathbf{z}, \mathbf{u}, \mathbf{y}(\mathbf{u}, \mathbf{d})) = \mathbf{r}^{\mathrm{sp}}, \qquad \forall\ \mathbf{d} \in \mathcal{D} \\ &\quad \mathbf{y}^{\mathrm{L}} \leq \mathbf{y}(\mathbf{u}, \mathbf{d}) \leq \mathbf{y}^{\mathrm{U}}, \qquad \forall\ \mathbf{d} \in \mathcal{D} \\ &\quad \mathbf{u}^{\mathrm{L}} \leq \mathbf{u} \leq \mathbf{u}^{\mathrm{U}}. \end{aligned} \tag{5}$$

This formulation corresponds to a mixed integer nonlinear semi-infinite optimization problem. Feasible values of the decision variables $\mathbf{z}$ and $\mathbf{r}^{\mathrm{sp}}$ require that for each disturbance $\mathbf{d} \in \mathcal{D}$, there is an input $\mathbf{u}$, such that the constraints are satisfied. Note that Problem (5) is the steady-state version of the closed-loop dynamic back-off problem presented in Bahri et al.[8]

2.3. Self-Optimizing Control. The self-optimizing control (SOC) approaches proposed in the literature are based on the idea of selecting the controlled variables so as to minimize the economic loss of the controlled plant with respect to optimal

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plant operation in the presence of disturbances.[26,28] This loss is given by:

$$L(\mathbf{z}, \mathbf{d}) = J(\mathbf{u}(\mathbf{z}, \mathbf{d}), \mathbf{d}) - J(\mathbf{u}^*(\mathbf{d}), \mathbf{d}) \tag{6}$$

where $\mathbf{u}(\mathbf{z},\mathbf{d})$ is the input reached at steady state by the controlled plant using the control structure $\mathbf{z}$, and $\mathbf{u}^*(\mathbf{d})$ is the optimal input obtained by solving Problem (3).

Most SOC approaches select as controlled variables linear combinations of the input and output variables. In this case, the vector $\mathbf{z}$ that determines the choice of the control structure includes the coefficients of the linear combinations, and the controlled variables $\mathbf{r} \in \mathbb{R}^{n_u}$ are given by:

$$\mathbf{r} = Q^T \begin{bmatrix} \mathbf{y}(\mathbf{u}, \mathbf{d}) \\ \mathbf{u} \end{bmatrix} \tag{7}$$

where $Q \in \mathbb{R}^{(n_u+n_y)\times n_u}$ is the linear combination matrix. In this paper, we will distinguish between classical control structures and linear combination control structures.

Definition 1 (classical control structure): A classical control structure is a square control structure that does not include linear combinations. In classical control structures, the vector $\mathbf{z}$ includes binary variables only, and the columns of matrix Q are unit vectors with exactly one element equal to one and the rest of elements equal to zero, while the rows in Q are either unit or zero vectors.

Definition 2 (linear combination control structure): A linear combination control structure is a (square) control structure that selects as controlled variable at least one linear combination of output (and input) variables or fixes at least one linear combination of input variables. In these control structures, at least one column of matrix Q has more than one element different from zero.

2.3.1. Null Space Method. The null space method[30] is a good method for explaining why linear combinations of output and input variables are selected as controlled variables in SOC approaches. For this purpose, the consideration of an unconstrained problem will suffice.

The NCO of the unconstrained problem $\min_{\mathbf{u}} J(\mathbf{u},\mathbf{d})$ is that the gradient be equal to zero at a solution point; that is, $\frac{\partial J}{\partial \mathbf{u}}(\mathbf{u}, \mathbf{d}) = 0$. The first-order variation of this condition evaluated at the nominal optimum reads:

$$\left.\frac{\partial^2 J}{\partial \mathbf{u}^2}\right|_n \delta\mathbf{u} + \left.\frac{\partial^2 J}{\partial \mathbf{u}\partial \mathbf{d}}\right|_n \delta\mathbf{d} = \mathbf{0} \tag{8}$$

Assuming that $\mathbf{u}^*(\mathbf{d}_n)$ is a strict local minimum, the Hessian is non-singular, and we can write:

$$\delta\mathbf{u}^*(\mathbf{d}) = \mathbf{K}\delta\mathbf{d}, \quad \text{with } \mathbf{K} = -\left(\left.\frac{\partial^2 J}{\partial \mathbf{u}^2}\right|_n\right)^{-1} \left.\frac{\partial^2 J}{\partial \mathbf{u}\partial \mathbf{d}}\right|_n \tag{9}$$

In turn, the first-order variation of the output variables is given by:

$$\delta\mathbf{y} = \left.\frac{\partial \mathbf{y}}{\partial \mathbf{u}}\right|_n \delta\mathbf{u} + \left.\frac{\partial \mathbf{y}}{\partial \mathbf{d}}\right|_n \delta\mathbf{d} \tag{10}$$

Using Problems (9) and (10), we can write:

$$\begin{bmatrix} \delta\mathbf{y} \\ \delta\mathbf{u} \end{bmatrix} = \mathbf{S}\delta\mathbf{d} \quad \text{with } \mathbf{S} = \begin{bmatrix} \left.\frac{\partial \mathbf{y}}{\partial \mathbf{u}}\right|_n \mathbf{K} + \left.\frac{\partial \mathbf{y}}{\partial \mathbf{d}}\right|_n \\ \mathbf{K} \end{bmatrix} \tag{11}$$

Let us assume that $\mathbf{S} \in \mathbb{R}^{(n_y+n_u)\times n_d}$ is full column rank, and let the columns in $\mathcal{N} \in \mathbb{R}^{(n_y+n_u)\times n_u}$ be a set of n_u orthonormal vectors that lie in the left null space of $\mathbf{S}$. Hence, $\mathcal{N}^T\mathbf{S} = \mathbf{0}$, and from (11), we have:

$$\delta\mathbf{r} = \mathcal{N}^T \begin{bmatrix} \delta\mathbf{y} \\ \delta\mathbf{u} \end{bmatrix} = \mathcal{N}^T\mathbf{S}\delta\mathbf{d} = \mathbf{0} \tag{12}$$

The null space method consists of selecting the combination matrix $Q = \mathcal{N}$ and controlling $\delta\mathbf{r} = \mathbf{0}$ by means of feedback controllers.[30] Notice that the dimension of the null space of $\mathbf{S}$ should be greater than or equal to n_u, which requires $n_y + n_u - n_d \geq n_u$. This last inequality reduces to $n_y \geq n_d$. That is, the number of measured output variables should be greater than or equal to the number of disturbances.[34] The null space method enforces local optimality. Indeed, using the first-order variation given by (10), it can be shown (under mild conditions) that enforcing $\delta\mathbf{r} = \mathbf{0}$ results in $\delta\mathbf{u} = \mathbf{K}\delta\mathbf{d}$ at steady state.[31]

2.3.2. Average Loss Methods. The so-called average loss methods[29,36−38] aim at selecting the controlled variables that minimize the expected value (or the average value) of the economic loss for a given disturbance set $\mathcal{D}$. The expected loss is given by:

$$L_{\text{exp}}(\mathbf{z}) = \underset{\mathbf{d}\in\mathcal{D}}{\mathrm{E}}\{\mathrm{J}(\mathbf{u}(\mathbf{z}, \mathbf{d}), \mathbf{d}) - \mathrm{J}(\mathbf{u}^*(\mathbf{d}), \mathbf{d})\} \tag{13}$$

3. STEADY-STATE BACK-OFF APPROACH WITH AVERAGE COST MINIMIZATION

In this section, we consider two alternative steady-state back-off problems based on the minimization of the average cost. The first problem consists in an MINLP formulation that determines the best classical control structure, while the second problem computes an optimal linear combination control structure by solving an NLP.

Remark 1 (expected loss versus expected cost): Let us consider the expected loss (13) used in the SOC. We have:

$$\begin{aligned} &\underset{\mathbf{d}\in\mathcal{D}}{\mathrm{E}}\{\mathrm{J}(\mathbf{u}(\mathbf{z}, \mathbf{d}), \mathbf{d}) - \mathrm{J}(\mathbf{u}^*(\mathbf{d}), \mathbf{d})\} \\ &\quad = \underset{\mathbf{d}\in\mathcal{D}}{\mathrm{E}}\{\mathrm{J}(\mathbf{u}(\mathbf{z}, \mathbf{d}), \mathbf{d})\} - \underset{\mathbf{d}\in\mathcal{D}}{\mathrm{E}}\{\mathrm{J}(\mathbf{u}^*(\mathbf{d}), \mathbf{d})\} \end{aligned} \tag{14}$$

Since the second expectation in the right side is a constant that does not depend on the control structure, it follows that, for the purpose of control structure selection, minimizing the expected loss is equivalent to minimizing the expected cost.

3.1. Selection of the Best Classical Control Structure.

The classical control structure selection problem can be written (without simplifications or approximations) as follows:

$$\begin{aligned} \min_{\mathbf{z},\mathbf{r}^{sp}} \; & \underset{\mathbf{d}\in\mathcal{D}}{\mathrm{E}}\{J(\mathbf{u}, \mathbf{d})\} \\ \text{s.t. } & \mathbf{r}(\mathbf{z}, \mathbf{u}, \mathbf{y}(\mathbf{u}, \mathbf{d})) = \mathbf{r}^{sp}(\mathbf{z}), \quad \forall\, \mathbf{d} \in \mathcal{D} \\ & \mathbf{y}^L \leq \mathbf{y}(\mathbf{u}, \mathbf{d}) \leq \mathbf{y}^U, \quad \forall\, \mathbf{d} \in \mathcal{D} \\ & \mathbf{u}^L \leq \mathbf{u} \leq \mathbf{u}^U \end{aligned} \tag{15}$$

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Note that the difference between this problem and the closed-loop steady-state back-off Problem (5) is that the expected cost is minimized instead of minimizing the cost for the nominal disturbance values.

As will be illustrated by means of the case studies in section 5, in steady-state back-off approaches minimizing the nominal cost is meaningful and beneficial if the optimal operating point is located at the intersection of the active constraints. However, if the solution is not completely determined by the active constraints, minimizing the nominal cost is of little value for selecting controlled variables for the unconstrained degrees of freedom that are left after controlling all the active constraints. However, minimizing the average cost permits us to select these additional controlled variables with self-optimizing properties.

In subsections 1.2 and 2.3, we reviewed self-optimizing control strategies. These methods focus on selecting controlled variables precisely for the remaining degrees of freedom that are left after controlling the active constraints. Many of these methods propose to minimize the average optimality loss in the presence of disturbances. Remark 1 implies that minimizing the average cost is similar to minimizing the average loss, which means that the back-off Problem (15) is also a self-optimizing control problem. Indeed, if in Problem (15) there are no active constraints, the problem still selects the control structure that minimizes the average cost in the presence of disturbances, which relates it to average-loss self-optimizing control methods.

3.1.1. Formulation as an MINLP. The vector of binary variables $\mathbf{z}$ that determines the control structure, and the vector of setpoint values $\mathbf{r}^{\mathrm{sp}}$ for the output and input variables, are parametrized as follows:

$$\mathbf{z} = \begin{bmatrix} \mathbf{z}^{\mathrm{O}} \\ \mathbf{z}^{\mathrm{I}} \end{bmatrix}, \quad \mathbf{z}^{\mathrm{O}} \in \mathbb{B}^{n_y}, \quad \mathbf{z}^{\mathrm{I}} \in \mathbb{B}^{n_u} \tag{16}$$

$$\mathbf{r}^{\mathrm{sp}} = \begin{bmatrix} \mathbf{y}^{\mathrm{sp}} \\ \mathbf{u}^{\mathrm{sp}} \end{bmatrix}, \quad \mathbf{y}^{\mathrm{sp}} \in \mathbb{R}^{n_y}, \quad \mathbf{u}^{\mathrm{sp}} \in \mathbb{R}^{n_u} \tag{17}$$

The binary components with values equal to one in vectors $\mathbf{z}^{\mathrm{O}}$ and $\mathbf{z}^{\mathrm{I}}$ correspond to the selected controlled output variables and the fixed input variables, respectively. The remaining components in $\mathbf{z}^{\mathrm{I}}$ with values equal to zero correspond to the selected manipulated variables.

Problem (15) is approximated by considering a finite number of disturbance values (scenarios). Let $\hat{\mathcal{D}}$ be a representative discretization of dimension N of the disturbance set $\mathcal{D}$; that is, $\hat{\mathcal{D}} = \{\mathbf{d}_1, ..., \mathbf{d}_N\}$. For convenience, we define the following index sets:

$$\mathcal{U} = \{1, 2, ..., n_u\}, \quad \mathcal{Y} = \{1, 2, ..., n_y\},$$
$$\mathcal{K} = \{1, 2, ..., N\}$$

The classical control structure selection problem is formulated as an MINLP as follows:

$$\min_{\mathbf{z}, \mathbf{r}^{\mathrm{sp}}, \mathbf{u}} \sum_{k=1}^{N} p_k J(\mathbf{u}_k, \mathbf{d}_k) \tag{18a}$$

$$\text{s.t.} \quad \sum_{i=1}^{n_y} z_i^{\mathrm{O}} + \sum_{j=1}^{n_u} z_j^{\mathrm{I}} = n_u \tag{18b}$$

$$y_i^{\mathrm{L}} z_i^{\mathrm{O}} \le y_i^{\mathrm{sp}} \le y_i^{\mathrm{U}} z_i^{\mathrm{O}}, \quad \forall\, i \in \mathcal{Y} \tag{18c}$$

$$u_j^{\mathrm{L}} z_j^{\mathrm{I}} \le u_j^{\mathrm{sp}} \le u_j^{\mathrm{U}} z_j^{\mathrm{I}}, \quad \forall\, j \in \mathcal{U} \tag{18d}$$

$$y_i^{\mathrm{L}}(1 - z_i^{\mathrm{O}}) \le y_i(\mathbf{u}_k, \mathbf{d}_k) - y_i^{\mathrm{sp}} \le y_i^{\mathrm{U}}(1 - z_i^{\mathrm{O}}), \quad \forall\, i \in \mathcal{Y}, k \in \mathcal{K} \tag{18e}$$

$$u_j^{\mathrm{L}}(1 - z_j^{\mathrm{I}}) \le u_{j,k} - u_j^{\mathrm{sp}} \le u_j^{\mathrm{U}}(1 - z_j^{\mathrm{I}}), \quad \forall\, j \in \mathcal{U}, k \in \mathcal{K} \tag{18f}$$

which is similar to the formulation proposed by Kookos.[20] (The main difference is that Kookos[20] considers the presence of measured and unmeasured disturbances, and the setpoints are computed as optimal polinomial functions of the measured disturbances. In Problem (18), the setpoints are constant, which can be seen as a special case of the formulation by Kookos.[20]) The expectation in the objective function is replaced by a weighted summation over the specified set of disturbance scenarios, where p_k are the weights for each disturbance scenario. If the disturbance realizations are uniformly distributed in $\mathcal{D}$, and $\hat{\mathcal{D}}$ is a uniform discretization of $\mathcal{D}$, then we take $p_k = \frac{1}{N}$ for $k = 1, ..., N$. Equation (18b) sets the total number of fixed variables equal to the number of inputs. The number of binary variables equal to one in $\mathbf{z}^{\mathrm{O}}$ defines the dimension of the control system (number of control loops). Note that the control problem is always square; that is, the number of manipulated variables is equal to the number of controlled output variables. By means of (18c) and (18d), the setpoints for the selected controlled output variables and fixed inputs are constrained to be within their boundary values, and if the variables are not controlled or fixed, their setpoints are set arbitrarily to zero. The constraints (18e) and (18f) force the controlled outputs and fixed inputs to match their setpoint values, while the uncontrolled outputs and manipulated inputs respect their respective boundary values for all disturbance scenarios $\mathbf{d}_k \in \hat{\mathcal{D}}$.

Remark 2. The steady-state back-off problem with nominal cost minimization (5) can be formulated as an MINLP in a similar way by replacing the average cost in (18a) by the nominal cost $J(\mathbf{u}_n, \mathbf{d}_n)$. A similar formulation can be found in Kookos and Perkins.[18]

3.1.2. Additional Constraints. 3.1.2.1. Fixed Number of Control Loops. Problem (18) can be solved for a fixed number of control loops $n_q \in \mathbb{I}^+$, $1 \le q \le \min\{n_y, n_u\}$, by adding the following constraint:

$$\sum_{i=1}^{n_y} z_i^{\mathrm{O}} = n_q \tag{19}$$

3.1.2.2. Input–Output Pairing Based on the RGA Matrix. In the context of control structure design, Braccia et al.[39] proposed to bound the relative gains of the relative gain array (RGA) to ensure that for the selected control structure there exists an input-output pairing that results in an acceptable degree of interaction when decentralized control is implemented.

Let $G \in \mathbb{R}^{n_y \times n_u}$ be the full input-output gain matrix of the open-loop system and $G_s(\mathbf{z}) \in \mathbb{R}^{n_q \times n_q}$ be the square submatrix

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determined by the selected controlled output variables (y_i for which $z_i^O = 1$) and the manipulated variables (u_j for which $z_j^I = 0$). The approach aims to evaluate the following constraints:[39]

$$\Lambda(\mathbf{z}) = G_s(\mathbf{z}) \otimes [G_s^{-1}(\mathbf{z})]^T \tag{20a}$$

$$\Lambda_p(\mathbf{z}, Z^p) = \Lambda(\mathbf{z}) \otimes Z^p(\mathbf{z}) \tag{20b}$$

$$\delta^L \leq \sum_{j=1}^{n_q} \lambda_{p,i,j}(\mathbf{z}, Z^p(\mathbf{z})) \leq \delta^U, \quad i = 1, ..., n_q \tag{20c}$$

$$\sum_{i=1}^{n_q} z_{i,j}^p = \sum_{j=1}^{n_q} z_{i,j}^p = 1 \tag{20d}$$

where $\Lambda(\mathbf{z})$ is the relative gain array corresponding to control structure $\mathbf{z}$; $Z^p \in \mathbb{B}^{n_q \times n_q}$ is a matrix of binary decision variables that determines the input−output pairing; the matrix $\Lambda_p \in \mathbb{R}^{n_q \times n_q}$ contains the elements of Λ selected by Z^p and zeros elsewhere; $\lambda_{p,i,j}$ are the elements of Λ_p, and $z_{i,j}^p$ are the elements of Z^p. In (20c), the lower and upper bounds on the relative gains, δ^L and δ^U, are design parameters that allow us to enforce a desired degree of interaction in a decentralized control structure.

Since Problem (18) uses a nonlinear model of the system, we propose to apply the constraints (20) by linearizing the model at the nominal optimum. That is, we select $G = \left.\frac{\partial \mathbf{y}}{\partial \mathbf{u}}\right|_n$ as the steady-state gain matrix computed at the nominal optimum $\mathbf{u}^*(\mathbf{d}_n)$. In general, this does not guarantee that the bounds (20c) will be satisfied for disturbance values different from the nominal ones or when we operate far from the nominal optimum due to the presence of constraint back-offs. In practice, however, evaluating these bounds at the nominal optimum already permits us to discard some inappropriate control structures.

Braccia et al.[39] proposed a reformulation of (20) as a set of linear constraints only. Next, we adapt this reformulation so that the resulting constraints conform to Problem (18). The reformulation requires introducing the following variables and parameters:

Continuous variables: inverse closed-loop gain matrix $\tilde{G} \in \mathbb{R}^{n_u \times n_y}$ with elements $\tilde{g}_{j,i}$; auxiliary matrix $\tilde{B} \in \mathbb{R}^{n_y \times n_y}$ with elements $\tilde{b}_{l,i}$; auxiliary matrix $\Lambda^r \in \mathbb{R}^{n_y \times n_u}$ with elements $\lambda_{i,j}^r$.

Binary variables: matrix $Z^{IO} \in \mathbb{B}^{n_y \times n_u}$ with elements $z_{i,j}^{IO}$.

Parameters: open-loop gain matrix $G \in \mathbb{R}^{n_y \times n_u}$ with elements $g_{i,j}$; big M values; lower RGA bound δ^L and upper bound δ^U.

These additional variables and parameters are included in Problem (18) together with the following linear constraints:

$$-M(1 - z_j^I) \leq \tilde{g}_{j,i} \leq M(1 - z_j^I), \quad \forall\, j \in \mathcal{U}, i \in \mathcal{Y} \tag{21a}$$

$$-M(z_i^O) \leq \tilde{g}_{j,i} \leq M(z_i^O), \quad \forall\, j \in \mathcal{U}, i \in \mathcal{Y} \tag{21b}$$

$$-M(2 - z_l^O - z_i^O) \leq \tilde{b}_{l,i} \leq M(2 - z_l^O - z_i^O), \quad \forall\, l \in \mathcal{Y}, i \in \mathcal{Y} \tag{21c}$$

$$\sum_j g_{l,j}\tilde{g}_{j,i} = \tilde{b}_{l,i} + I_{l,i} z_i^O, \quad \forall\, l \in \mathcal{Y}, i \in \mathcal{Y} \tag{21d}$$

$$\sum_j z_{i,j}^{IO} = z_i^O, \quad \forall\, i \in \mathcal{Y} \tag{21e}$$

$$\sum_i z_{i,j}^{IO} = (1 - z_j^I), \quad \forall\, j \in \mathcal{U} \tag{21f}$$

$$-M(1 - z_{i,j}^{IO}) \leq \lambda_{i,j}^r - g_{i,j}\tilde{g}_{j,i} \leq M(1 - z_{i,j}^{IO}), \quad \forall\, i \in \mathcal{Y}, j \in \mathcal{U} \tag{21g}$$

$$\delta^L z_{i,j}^{IO} \leq \lambda_{i,j}^r \leq \delta^U z_{i,j}^{IO}, \quad \forall\, i \in \mathcal{Y}, j \in \mathcal{U} \tag{21h}$$

As mentioned, $G_s(\mathbf{z})$ is the (square) submatrix of G obtained for a given control structure $\mathbf{z}$. Let $\tilde{G}_s(\mathbf{z})$ be the corresponding submatrix of $\tilde{G}$. Equations (21a) and (21b) set to zero all of the elements of matrix $\tilde{G}$ except for those corresponding to the selected submatrix $\tilde{G}_s(\mathbf{z})$. Consider the square matrix $B = G\tilde{G}$ and let $B_s(\mathbf{z})$ be the submatrix of B corresponding to the selected controlled output variables $\mathbf{z}^O$. Equations (21c) and (21d) are used to set $G_s(\mathbf{z})\tilde{G}_s(\mathbf{z}) = B_s(\mathbf{z}) = \mathbf{I}$. This approach allows us to obtain the inverse matrix $\tilde{G}_s(\mathbf{z})$ for any control structure $\mathbf{z}$ by means of linear constraints. By means of eq (21d), we have $G\tilde{G} = B = \tilde{B} + \text{diag}(\mathbf{z}^O)$. Equations (21e) and (21f) are used to build the input-output pairing matrix Z^{IO}. Note that matrix $Z^p(\mathbf{z})$ in (20) is the square submatrix of Z^{IO} corresponding to the control structure $\mathbf{z}$. In eq (21g), the elements of the RGA matrix are computed and allocated in the elements $\lambda_{i,j}^r$ of matrix Λ^r based on the pairing selection Z^{IO}. These elements are restricted to satisfy the defined bounds in (21h). Note that Λ_p in (20) is the square submatrix of Λ^r corresponding to the control structure $\mathbf{z}$ and the pairing Z^{IO}.

A similar formulation for computing the RGA matrix by means of linear equations was proposed by Kookos and Perkins.[40] A difference with the work of Kookos and Perkins[40] is that they determine the input−output pairing and the RGA matrix for a given set of controlled variables, while our formulation determines the input−output pairing and the RGA matrix for any allowed set of controlled variables. The following example illustrates the implementation of constraints (21) for a given control structure.

Example 1 (Bounds on RGA Matrix): Let us consider a system with four inputs ($n_u = 4$) and six measured outputs ($n_y = 6$) and consider the control structure defined by $\mathbf{z}^O = [0\ 1\ 0\ 1\ 0\ 0]$ and $\mathbf{z}^I = [0\ 1\ 1\ 0]$. For this control structure of size $n_q = 2$, the CVs are y_2 and y_4, and the MVs are u_1 and u_4. By means of (21a) and (21b), the matrix $\tilde{G}$ takes the form:

$$\tilde{G} = \begin{bmatrix} 0 & \tilde{g}_{1,2} & 0 & \tilde{g}_{1,4} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \tilde{g}_{4,2} & 0 & \tilde{g}_{4,4} & 0 & 0 \end{bmatrix}$$

The matrix multiplication $G\tilde{G} = B$ gives

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$$B = \begin{bmatrix} 0 & b_{1,2} & 0 & b_{1,4} & 0 & 0 \\ 0 & b_{2,2} & 0 & b_{2,4} & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & b_{6,2} & 0 & b_{6,4} & 0 & 0 \end{bmatrix}$$

with $b_{i,j} = g_{i,1}\tilde{g}_{1,j} + g_{i,4}\tilde{g}_{4,j}$. This matrix captures the information on the selected subprocess multiplication in the elements $b_{2,2}$, $b_{2,4}$, $b_{4,2}$, and $b_{4,4}$. To see this, consider the submatrices G_s, $\tilde{G}_s$, and B_s for the selected CVs and MVs:

$$G_s = \begin{bmatrix} g_{2,1} & g_{2,4} \\ g_{4,1} & g_{4,4} \end{bmatrix}, \quad \tilde{G}_s = \begin{bmatrix} \tilde{g}_{1,2} & \tilde{g}_{1,4} \\ \tilde{g}_{4,2} & \tilde{g}_{4,4} \end{bmatrix},$$

$$G_s\tilde{G}_s = B_s = \begin{bmatrix} b_{2,2} & b_{2,4} \\ b_{4,2} & b_{4,4} \end{bmatrix}$$

The matrix multiplication $G_s\tilde{G}_s$ is performed in (21d) with $B = \tilde{B} + \mathrm{diag}(\mathbf{z}^{O})$. The restrictions on $\tilde{B}$ in (21c) imply that:from where we can see that $B_s = \mathbf{I}$, and thus, $\tilde{G}_s$ is the inverse of G_s.

$$B = \begin{bmatrix} 0 & b_{1,2} & 0 & b_{1,4} & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & b_{3,2} & 0 & b_{3,4} & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & b_{5,2} & 0 & b_{5,4} & 0 & 0 \\ 0 & b_{6,2} & 0 & b_{6,4} & 0 & 0 \end{bmatrix}$$

The pairing determined by the binary matrix $\mathbf{z}^{IO}$ has two alternatives based on the CS defined by $\mathbf{z}^{O}$ and $\mathbf{z}^{I}$:

$$Z_a^{IO} = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}, \quad or \quad Z_b^{IO} = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

These two alternatives are generated via eqs (21e) and (21f), and it means that for Z_a^{IO}, for example, the loops proposed are $y_2 - u_1$ and $y_4 - u_4$. The resulting RGA elements ($\lambda_{i,j}^r = g_{i,j}\tilde{g}_{j,i}$) are stored in the auxiliary matrix Λ^r via (21g), and their values are restricted to satisfy the predefined bounds in (21h). For example, for the pairing Z_a^{IO}, we get:

$$\begin{bmatrix} 0 & 0 & 0 & 0 \\ \delta^L & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \delta^L \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \le \Lambda_a^r = \begin{bmatrix} 0 & 0 & 0 & 0 \\ g_{2,1}\tilde{g}_{1,2} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & g_{4,4}\tilde{g}_{4,4} \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \le \begin{bmatrix} 0 & 0 & 0 & 0 \\ \delta^U & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \delta^U \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \quad (22)$$

3.1.3. Solution Strategy. The MINLP Problem (18) can be solved in GAMS using the available solvers such as BARON or others. However, the formulation might be difficult to solve for complex process models. The major limitation of Problem (18) comes from the nonlinearities and nonconvexities in the model equations used to compute the mappings $J(\mathbf{u},\mathbf{d})$ and $y_i(\mathbf{u},\mathbf{d})$, $i = 1, ..., n_y$. Additionally, the problem becomes cumbersome as the number of discretization scenarios grows.

Once the optimal CS $\mathbf{z}^*$ is determined, the next step is to select the controller interaction and technology, and the resulting plant-wide control system needs to be validated by means of stability, controllability and robustness tests, possibly requiring dynamic simulations. If the resulting CS $\mathbf{z}^*$ has been validated, it can be applied to the plant. Conversely, if the optimal CS is found to be unsuitable, an integer cut is introduced and Problem (18) is solved again until an appropriate CS is obtained.

In many cases, the use of a thick disturbance discretization in the MINLP problem is sufficient to reveal the correct optimal control structure. However, due to the approximation, the setpoints obtained might not be suitable. To avoid the risk of constraint violations for some disturbance scenarios, the setpoints should be recomputed by fixing the control structure $\mathbf{z}$ in Problem (18) to the optimal structure obtained and then solving Problem (18) as an NLP using a fine discretization of the disturbance set $\mathcal{D}$.

3.2. Selection of a Linear Combination Control Structure. The problem of selecting linear combinations of output and input variables as controlled variables can be formulated as follows:

$$\begin{aligned} &\min_{Q,\mathbf{r}^{sp}} \ \mathop{\mathrm{E}}_{\mathbf{d}\in\mathcal{D}} \{J(\mathbf{u}, \mathbf{d})\} \\ &\text{s.t. } \mathbf{r} = Q^T \begin{bmatrix} \mathbf{y}(\mathbf{u}, \mathbf{d}) \\ \mathbf{u} \end{bmatrix} = \mathbf{r}^{sp}, \quad \forall\, \mathbf{d} \in \mathcal{D} \\ &\quad \mathbf{y}^L \le \mathbf{y}(\mathbf{u}, \mathbf{d}) \le \mathbf{y}^U, \qquad \forall\, \mathbf{d} \in \mathcal{D} \\ &\quad \mathbf{u}^L \le \mathbf{u} \le \mathbf{u}^U, \end{aligned} \qquad (23)$$

where $\mathbf{r} \in \mathbb{R}^{n_u}$ are the controlled variables, $Q \in \mathbb{R}^{(n_u+n_y)\times n_u}$ is the linear combination matrix, and $\mathbf{r}^{sp} \in \mathbb{R}^{n_u}$ are the setpoint values.

3.2.1. Formulation as an NLP. Upon discretization of the disturbance set $\mathcal{D}$, Problem (23) can be approximated as an NLP:

$$\min_{Q,\mathbf{r}^{sp},\mathbf{u}} \sum_{k=1}^{N} p_k J(\mathbf{u}_k, \mathbf{d}_k) \qquad (24a)$$

$$\text{s.t. } Q^T \begin{bmatrix} \mathbf{y}(\mathbf{u}_k, \mathbf{d}_k) \\ \mathbf{u}_k \end{bmatrix} = \mathbf{r}^{sp}, \qquad \forall\, k \in \mathcal{K} \qquad (24b)$$

$$\mathbf{y}^L \le \mathbf{y}(\mathbf{u}_k, \mathbf{d}_k) \le \mathbf{y}^U, \qquad \forall\, k \in \mathcal{K} \qquad (24c)$$

$$\mathbf{u}^L \le \mathbf{u}_k \le \mathbf{u}^U, \qquad \forall\, k \in \mathcal{K} \qquad (24d)$$

The selection of a full matrix Q will in general lead to infinite solutions. This can be avoided by imposing a predefined structure and parametrization of matrix Q (examples of this will be seen in Subsections 5.1 and 5.2).

Remark 3: In the context of SOC, Yelchuru and Skogestad[41] formulated a mixed-integer optimization problem that finds the best subset of measurements for the linear combinations. Note that a similar approach could be implemented in Problem (24), which would then become an MINLP.

3.2.2. Additional Constraints. Optionally, one can add to Problem (24) the following constraint:

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$$Q^T\begin{bmatrix} G \\ \mathbf{I} \end{bmatrix} = T \tag{25}$$

where $G \in \mathbb{R}^{n_y \times n_u}$ is the input−output gain matrix of the open-loop system, evaluated at the nominal optimum, and $T \in \mathbb{R}^{n_u \times n_u}$ is the gain matrix imposed on the controlled process. In the SOC literature, T has been selected as the identity matrix[30,36] or as the square root of the cost Hessian[37,41] (to simplify a particular local SOC formulation). T may also be selected as any permutation of the identity matrix or in general as any well-conditioned matrix. The use of constraint (25) will be illustrated in section 5.3.

Notice that the RGA matrix for a linear combination control structure is given by $T \otimes [T^{-1}]^T$. Hence, the choice of an appropriate pairing between the manipulated variables and the controlled variables is determined by the choice of matrix T.

The inclusion of the constraint (25) is advantageous for three reasons: (i) it restricts the search space considerably; (ii) it enforces invertibility of the controlled process (at least at nominal conditions), which is linked with steady-state controllability; and (iii) it does not affect the optimal cost of Problem (24). This last assertion can be proved as follows. Let us assume that Q_1 with setpoints $\mathbf{r}_1^{\mathrm{sp}}$ is an optimal solution to Problem (24). Then, for any nonsingular matrix C, $Q^T = CQ_1^T$ with setpoints $\mathbf{r}^{\mathrm{sp}} = C\mathbf{r}_1^{\mathrm{sp}}$ is also an optimal solution with the same optimal cost. The gain matrix of the controlled process $B = Q_1^T[G; \mathbf{I}]$ should be invertible for steady-state controllability. Hence, if T is also non-singular, one can select the non-singular matrix $C = T(B)^{-1}$, such that $CB = T$.

4. APPROXIMATION AS AN MIQP

One of the major limitations of the MINLP Problem (18) is the difficulty to find the global optimum for nonconvex problems. The source of nonlinearities and nonconvexities in this problem comes from the functions $J(\mathbf{u},\mathbf{d})$ and $y_i(\mathbf{u},\mathbf{d})$, $i = 1, ..., n_y$. In this section, we circumvent this difficulty by approximating Problem (18) as a convex MIQP problem. Two alternative MIQP approximations will be proposed next. The first one, which we denote lugd-MIQP, is local in the inputs $\mathbf{u}$ and global in the disturbances $\mathbf{d}$, whereas the second one, denoted luld-MIQP, is local in both the inputs and the disturbances.

4.1. Global Disturbance MIQP.

For a given disturbance $\mathbf{d}_k \in \hat{\mathcal{D}}$, we consider the QP approximation used in successive quadratic programming (SQP) methods for solving NLP problems.[42,43] The QP approximation of the NLP Problem (3) at the optimal point $\mathbf{u}^*(\mathbf{d}_k)$ is given by:

$$\min_{\boldsymbol{\delta}\mathbf{u}_k} \left.\frac{\partial J}{\partial \mathbf{u}}\right|_k \boldsymbol{\delta}\mathbf{u}_k + \frac{1}{2}\boldsymbol{\delta}\mathbf{u}_k^T H_k \boldsymbol{\delta}\mathbf{u}_k \tag{26a}$$

$$\text{s.t. } y_i^{\mathrm{L}} \le y_{i,k} + \left.\frac{\partial y_i}{\partial \mathbf{u}}\right|_k \boldsymbol{\delta}\mathbf{u}_k \le y_i^U, \qquad i = 1, ..., n_y \tag{26b}$$

$$\mathbf{u}_k = \mathbf{u}^*(\mathbf{d}_k) + \boldsymbol{\delta}\mathbf{u}_k \tag{26c}$$

$$\mathbf{u}^{\mathrm{L}} \le \mathbf{u}_k \le \mathbf{u}^{\mathrm{U}} \tag{26d}$$

where $\left.\frac{\partial J}{\partial \mathbf{u}}\right|_k$ and $\left.\frac{\partial y_i}{\partial \mathbf{u}}\right|_k$ are evaluated at the optimal point $\mathbf{u}^*(\mathbf{d}_k)$, $y_{i,k} = y_i(\mathbf{u}^*(\mathbf{d}_k),\mathbf{d}_k)$, and H_k is a positive definite approximation of the Hessian of the Lagrangian function $\left.\frac{\partial^2 L}{\partial \mathbf{u}^2}\right|_k$, evaluated at $\mathbf{u}^*(\mathbf{d}_k)$. In this formulation, the output constraints are linearized at $\mathbf{u}^*(\mathbf{d}_k)$, and the curvature of the constraints is taken into account by using the Hessian of the Lagrangian function in the quadratic term of the objective function. Since the Hessian of the Lagrangian can be indefinite at a Karush−Kuhn−Tucker (KKT) point, we replace it by a positive semi-definite approximation matrix H_k to have a convex QP problem.

Several approaches are available for approximating the Lagrangian Hessian. The approach used in this work is based on the eigenvalue decomposition of the symmetric matrix $\left.\frac{\partial^2 L}{\partial \mathbf{u}^2}\right|_k$:

$$\left.\frac{\partial^2 L}{\partial \mathbf{u}^2}\right|_k = U_k D_k U_k^{\mathrm{T}}$$

with a diagonal matrix D_k and an orthonormal matrix U_k. Let D_k^+ be the matrix obtained from D_k by replacing the negative entries of D_k with zeros. The Hessian approximation H_k is obtained as:

$$H_k = U_k D_k^+ U_k^T$$

Based on the convex QP approximation (26), we use the following approximations for the functions $J(\mathbf{u},\mathbf{d})$ and $y_i(\mathbf{u},\mathbf{d})$:

$$\tilde{J}(\mathbf{u}_k, \mathbf{d}_k) = \left.\frac{\partial J}{\partial \mathbf{u}}\right|_k \boldsymbol{\delta}\mathbf{u}_k + \frac{1}{2}\boldsymbol{\delta}\mathbf{u}_k^{\mathrm{T}} H_k \boldsymbol{\delta}\mathbf{u}_k \tag{27a}$$

$$\tilde{y}_i(\mathbf{u}_k, \mathbf{d}_k) = y_{i,k} + \left.\frac{\partial y_i}{\partial \mathbf{u}}\right|_k \boldsymbol{\delta}\mathbf{u}_k, \qquad i = 1, ..., n_y \tag{27b}$$

Note that the zeroth-order term in the cost function in (27a) has been omitted because it does not affect the optimal solution. Using these function approximations, the following constraints should be added to Problem (18):

$$\mathbf{u}_n = \mathbf{u}^*(\mathbf{d}_n) + \boldsymbol{\delta}\mathbf{u}_n \tag{28a}$$

$$\mathbf{u}_k = \mathbf{u}^*(\mathbf{d}_k) + \boldsymbol{\delta}\mathbf{u}_k, \qquad k = 1, ..., N \tag{28b}$$

This way, the lugd-MIQP approximation of Problem (18) is obtained by implementing the following steps:

(i) For all disturbance scenarios $\mathbf{d}_k$, $k = 1, ..., N$, solve the NLP Problem (3) to obtain the corresponding optimal inputs $\mathbf{u}^*(\mathbf{d}_k)$, $k = 1, ..., N$.

(ii) Evaluate $y_{i,k}$ and $\left.\frac{\partial y_i}{\partial \mathbf{u}}\right|_k$ for $i = 1, ..., n_y$, $\left.\frac{\partial J}{\partial \mathbf{u}}\right|_k$, and the Hessian approximation H_k, at the optimal inputs $\mathbf{u}^*(\mathbf{d}_k)$, for all disturbance scenarios $\mathbf{d}_k$, $k = 1, ..., N$.

(iii) Replace $J(\mathbf{u}_k,\mathbf{d}_k)$ and $y_i(\mathbf{u}_k,\mathbf{d}_k)$ in Problem (18) by the approximations (27a) and (27b), respectively. Add the constraints for Problem (28) to Problem (18).

4.2. Local Disturbance MIQP.

To avoid the computational burden of having to solve the NLP Problem (3) for all disturbance scenarios, and having to evaluate the required gradient and Hessian information at all the solution points, we propose to further simplify the MIQP approximation of Problem (18) by considering the following approximation of the NLP Problem (3):

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$$\min_{\delta \mathbf{u}} \left.\frac{\partial J}{\partial \mathbf{u}}\right|_n \delta\mathbf{u} + \delta\mathbf{d}^T \left.\frac{\partial^2 J}{\partial \mathbf{d}\partial \mathbf{u}}\right|_n \delta\mathbf{u} + \frac{1}{2}\delta\mathbf{u}^T H_n \delta\mathbf{u} \tag{29a}$$

$$\text{s.t.} \quad y_i^L \le y_{i,n} + \left.\frac{\partial y_i}{\partial \mathbf{u}}\right|_n \delta\mathbf{u} + \left.\frac{\partial y_i}{\partial \mathbf{d}}\right|_n \delta\mathbf{d} + \delta\mathbf{d}^T \left.\frac{\partial^2 y_i}{\partial \mathbf{d}\partial \mathbf{u}}\right|_n \delta\mathbf{u} + \frac{1}{2}\delta\mathbf{d}^T \left.\frac{\partial^2 y_i}{\partial \mathbf{d}^2}\right|_n \delta\mathbf{d} \le y_i^U \tag{29b}$$

$$\mathbf{u} = \mathbf{u}^*(\mathbf{d}_n) + \delta\mathbf{u}, \quad \mathbf{d} = \mathbf{d}_n + \delta\mathbf{d} \tag{29c}$$

$$\mathbf{u}^L \le \mathbf{u} \le \mathbf{u}^U \tag{29d}$$

where the partial derivatives $\left.\frac{\partial J}{\partial \mathbf{u}}\right|_n$, $\left.\frac{\partial^2 J}{\partial \mathbf{d}\partial \mathbf{u}}\right|_n$, and $\left.\frac{\partial y_i}{\partial \mathbf{u}}\right|_n$, $\left.\frac{\partial y_i}{\partial \mathbf{d}}\right|_n$, $\left.\frac{\partial^2 y_i}{\partial \mathbf{d}\partial \mathbf{u}}\right|_n$, $\left.\frac{\partial^2 y_i}{\partial \mathbf{d}^2}\right|_n$, for $i = 1, ..., n_y$, are all evaluated at the nominal optimum of Problem (3), $\mathbf{u}^*(\mathbf{d}_n)$, and H_n is a positive definite approximation of the Hessian of the Lagrangian function $\left.\frac{\partial^2 L}{\partial \mathbf{u}^2}\right|_n$, evaluated at $\mathbf{u}^*(\mathbf{d}_n)$. Note that Problem (29) is quadratic and convex in terms of the inputs $\mathbf{u}$ (i.e., for $\delta\mathbf{d}$ fixed) and represents a local approximation of Problem (3) in terms of both the inputs and the disturbances.

Based on Problem (29), $\tilde{J}(\mathbf{u}_k,\mathbf{d}_k)$ and $\tilde{y}_i(\mathbf{u}_k,\mathbf{d}_k)$ are given by:

$$\tilde{J}(\mathbf{u}_k, \mathbf{d}_k) = \left.\frac{\partial J}{\partial \mathbf{u}}\right|_n \delta\mathbf{u}_k + \delta\mathbf{d}_k^T \left.\frac{\partial^2 J}{\partial \mathbf{d}\partial \mathbf{u}}\right|_n \delta\mathbf{u}_k + \frac{1}{2}\delta\mathbf{u}_k^T H_k \delta\mathbf{u}_k \tag{30a}$$

$$\tilde{y}_i(\mathbf{u}_k, \mathbf{d}_k) = y_{i,n} + \left.\frac{\partial y_i}{\partial \mathbf{u}}\right|_n \delta\mathbf{u}_k + \left.\frac{\partial y_i}{\partial \mathbf{d}}\right|_n \delta\mathbf{d}_k + \delta\mathbf{d}_k^T \left.\frac{\partial^2 y_i}{\partial \mathbf{d}\partial \mathbf{u}}\right|_n \delta\mathbf{u}_k + \frac{1}{2}\delta\mathbf{d}_k^T \left.\frac{\partial^2 y_i}{\partial \mathbf{d}^2}\right|_n \delta\mathbf{d}_k, \quad i = 1, ..., n_y \tag{30b}$$

The luld-MIQP approximation of Problem (18) is obtained by implementing the following steps:

(i) Solve the NLP Problem (3) for the nominal disturbance $\mathbf{d}_n$ to obtain the nominal optimum $\mathbf{u}^*(\mathbf{d}_n)$.

(ii) Evaluate the partial derivatives $\left.\frac{\partial J}{\partial \mathbf{u}}\right|_n$, $\left.\frac{\partial^2 J}{\partial \mathbf{d}\partial \mathbf{u}}\right|_n$, $\left.\frac{\partial y_i}{\partial \mathbf{u}}\right|_n$, $\left.\frac{\partial y_i}{\partial \mathbf{d}}\right|_n$, $\left.\frac{\partial^2 y_i}{\partial \mathbf{d}\partial \mathbf{u}}\right|_n$, $\left.\frac{\partial^2 y_i}{\partial \mathbf{d}^2}\right|_n$, for $i = 1, ...,n_y$, and the Hessian approximation H_n, at $\mathbf{u}^*(\mathbf{d}_n)$.

(iii) Replace $J(\mathbf{u}_k,\mathbf{d}_k)$ and $y_i(\mathbf{u}_k,\mathbf{d}_k)$ in Problem (18) by the approximations (30a) and (30b), respectively. Add the constraints (28) to Problem (18).

4.3. Quality of the Approximation and Implementation Aspects. The MIQP approximations presented in sections 4.1 and 4.2 may not lead to the optimal control structure of the original MINLP formulation Problem (18). However, in cases in which Problem (18) becomes computationally intractable, the MIQP approximations are much easier to solve and permit us to obtain a suboptimal solution. The quality of the approximation will depend on the particular application at hand, but in general, one can expect that the approximations will be locally good, for small disturbance variations.

In cases in which the set of active constraints changes with the disturbance values, and the constraints that become active or inactive are nonlinear, the local disturbance MIQP approximation may be inadequate because, in this local approach, the Hessian of the Lagrangian function computed at the nominal optimum is used for all disturbance scenarios. If, for any given disturbance scenario, the active set changes with respect to the active set at the nominal optimum, the Hessian of the Lagrangian may change significantly with respect to the nominal Hessian (this is not the case if the constraints that become active or inactive are input bounds or linear constraints because their Hessian is equal to zero). Hence, in the presence of changes in the active set we recommend to use the global disturbance MIQP approximation.

5. CASE STUDIES

5.1. Linear System. We consider a linear system similar to the one proposed in Marchetti et al.[44] The steady-state behavior of the plant is described by the following system:

$$\mathbf{y}(\mathbf{u}, \mathbf{d}) = \mathbf{y}_s - A_s\mathbf{u} - D_s\mathbf{d}$$

with

$$A_s = \begin{bmatrix} -1.00 & 1.00 \\ -1.00 & -1.00 \\ -1.60 & 0.24 \end{bmatrix}, \quad D_s = \begin{bmatrix} -0.2702 & 0 & 0 \\ 0 & 0.3003 & 0 \\ 0 & 0 & -0.3809 \end{bmatrix},$$

$$\mathbf{y}_s = \begin{bmatrix} -0.35 \\ -1.00 \\ -1.10 \end{bmatrix}$$

which consists of two input variables, $\mathbf{u} = [u_1, u_2]^T$, three measured outputs, $\mathbf{y} = [y_1, y_2, y_3]^T$, and three unmeasured disturbances, $\mathbf{d} = [d_1, d_2, d_3]^T$. The objective is to maximize the linear function $J(\mathbf{u}) = 6.85u_1 + 2.95u_2$ subject to constraints on the output variables. Two optimization problems will be considered. Problem A includes constraints on the outputs y_1 and y_2, while Problem B includes constraints on the three outputs:

Problem A

$$\max_{\mathbf{u}} \; 6.85u_1 + 2.95u_2$$
$$\text{s.t.} \; y_1(\mathbf{u}, d_1) \le 0, \quad y_2(\mathbf{u}, d_2) \le 0, \quad 0 \le u_1, u_2 \le 1.$$

Problem B

$$\max_{\mathbf{u}} \; 6.85u_1 + 2.95u_2$$
$$\text{s.t.} \; \mathbf{y}(\mathbf{u}, \mathbf{d}) \le 0, \quad 0 \le u_1, u_2 \le 1.$$

In this example, each disturbance affects independently each output variable. The nominal disturbance values are zero; that is, $\mathbf{d}_n = \mathbf{0}$. The disturbances are assumed to be uniformly distributed in the following ranges: $-1 \le d_1 \le 1$, $-1 \le d_2 \le 1$, and $-0.1 \le d_3 \le 0.1$. The contour maps for Problems A and B are shown in Figure 1. The colored area corresponds to the feasible region for the nominal disturbance values for both problems. Point **a** is the nominal optimum for both problems; that is, $\mathbf{a} = \mathbf{u}^*(\mathbf{d}_n)$. Note that the constraints on y_1 and y_2 are active at the nominal optimum. Point **b** is the solution to the open-loop steady-state back-off problem. This point corresponds to the optimum for the worst-case disturbance realization $\mathbf{d} = [1,-1]^T$.

For this linear system, Problem (18) and its nominal cost counterpart become MILPs, and as such, we solve them in GAMS using the solver CPLEX. Each solution is obtained in less than a second of CPU time. The N disturbance scenarios are obtained via a grid discretization of the disturbance set with $d_{1,k} \in \{-1{:}\ 0.5{:}\ 1\}$, $d_{2,k} \in \{-1{:}\ 0.5{:}\ 1\}$, and $d_{3,k} \in \{-0.1{:}\ 0.05{:}\ 0.1\}$. In fact, for a linear system, it would be

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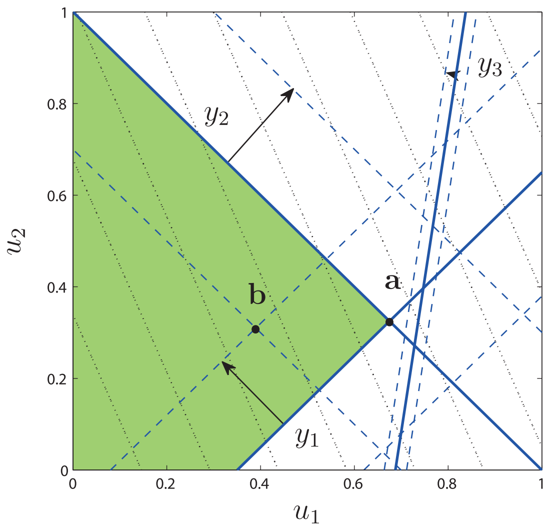

Figure 1. Contour maps for Problems A and B. Colored area: feasible region for the nominal disturbances. Thick solid lines: boundaries of the output constraints for the nominal disturbances. Dashed lines: boundaries of the output constraints for the extreme values of the disturbances. Dotted lines: contours of the objective function. Point **a**: nominal optimum. Point **b**: solution to the open-loop steady-state back-off problem. The arrows indicate the constraint movements produced by changing the values of disturbances d_i, $i = 1, 2, 3$ from 0 to 1.

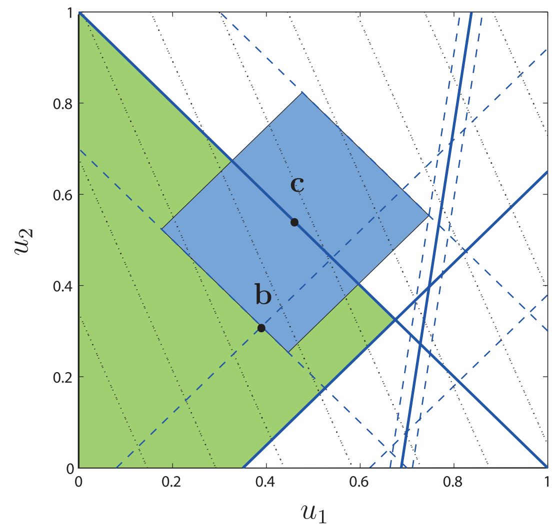

Figure 2. Contour maps for Problem B. Blue area: operating region for the optimal control structure CS1. Point **b**: solution to the open-loop steady-state back-off problem. Point **c**: nominal operating point for the control structure CS1.

sufficient to evaluate the constraints at the extreme values of the disturbances to guarantee feasibility. Because the disturbance ranges are centered at the nominal values and the problem is linear, the back-off problem with average cost minimization gives the same results as the back-off problem with nominal cost minimization in this example.

5.1.1. Control Structure Selection for Problem A. In the case of Problem A, the constraints on y_1 and y_2 are both active for the nominal disturbance values and for all possible realizations of the disturbances d_1 and d_2. Hence, in this problem, the optimal operating point is at the intersection of the active constraints, and the set of active constraints does not change with the disturbance values. The optimal control structure obtained for both, the steady-state back-off problems with nominal and average cost minimization, is to control both active constraints (the outputs y_1 and y_2) with zero back-offs, i.e., with setpoints $y_1^{sp} = y_2^{sp} = 0$.

5.1.2. Control Structure Selection for Problem B. Problem B includes constraints on the three output variables, and it becomes clear from Figure 1 that there are many disturbance scenarios for which the constraint on y_3 becomes active, while the constraint on y_1 becomes inactive. Hence, in this problem, the optimal operating point is at the intersection of the active constraints, but the set of active constraints changes depending on the disturbance values. The optimal control structure obtained for both, the steady-state back-off problems with nominal and average cost minimization, which we denote CS1, is to control the output y_2 with zero back-off ($y_2^{sp} = 0$), and the output y_1 with a significant back-off of 0.427 ($y_1^{sp} = -0.427$). The nominal operating point and the operating region for this control structure are shown in Figure 2. Note that the back-off on y_1 is selected as the smallest back-off such that the constraint on y_3 never becomes violated by controlling y_1 and y_2.

In this low-dimension problem, there are only ten possible classical control structures, which are ordered in Table 2 according to their optimal value. The control structure CS5 corresponds to the open-loop solution. Note that the control structures CS6 to CS9 perform worse than the open-loop solution, while CS10 is infeasible. The optimal setpoints obtained via optimization for each control structure are given in Table 3.

Table 2. CSs for the Linear System

	$\mathbf{z}^O$			$\mathbf{z}^I$			
CS	y_1	y_2	y_3	u_1	u_2	J_n ($N = 125$)	J_{av} ($N = 125$)
CS1	1	1	0	0	0	4.750	4.750
CS2	0	1	1	0	0	4.542	4.542
CS3	0	1	0	0	1	4.470	4.470
CS4	0	1	0	1	0	4.470	4.470
CS5	0	0	0	1	1	3.584	3.584
CS6	0	0	1	0	1	3.421	3.421
CS7	1	0	0	0	1	2.787	2.787
CS8	0	0	1	1	0	2.497	2.497
CS9	1	0	0	1	0	1.888	1.888
CS10	1	0	1	0	0	infeasible	infeasible

Because many dynamic back-off approaches fix the input variables that are not selected as manipulated variables at their nominal optimal values,[14,15,17,22] it is interesting to see the effect this has from the steady-state perspective. Let us consider, for instance, the control structure CS3 from Table 2, for which the

Table 3. Calculated Setpoints for the Linear System

	$\mathbf{r}^{sp}$				
CS	y_1	y_2	y_3	u_1	u_2
CS1	−0.427	0.000	–	–	–
CS2	–	0.000	−0.589	–	–
CS3	–	0.000	–	–	0.610
CS4	–	0.000	–	0.397	–
CS5	–	–	–	0.389	0.310
CS6	–	–	−0.589	–	0.310
CS7	0.000	–	–	–	0.039
CS8	–	–	−0.805	0.231	–
CS9	−0.461	–	–	0.159	–

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operating line and the nominal point **s** are shown in Figure 3. If, instead of fixing u_2 at the optimal value of 0.61, we fix it at the

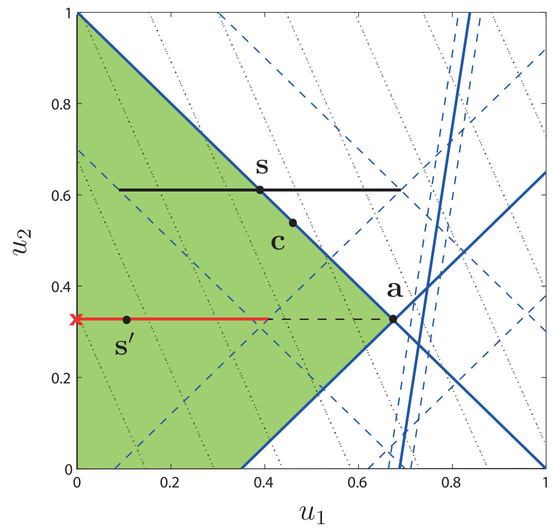

Figure 3. Contour maps for Problem B. Thick black segment: operating line for control structure CS3. Thick red segment: operating line for CS3 with u_2 fixed at its nominal optimum value. Point **a**: nominal optimum. Point **c**: nominal operating point for CS1. Point **s**: nominal operating point for CS3. Point **s**′: nominal operating point for CS3 with $u_2 = u_2^*(\mathbf{d}_n)$.

nominal value of 0.325, a considerable back-off of size 0.5705 is required for the controlled variable y_2 to maintain feasibility for all disturbance scenarios. Hence, the nominal point **s** moves to point **s**′ in Figure 3, which is highly suboptimal. Even if this CS would be feasible in practice, note that the input u_1 becomes saturated for many disturbance values, which means that we lose control on y_2. Because input saturation effects are not contemplated in Problem (18), this CS will be infeasible for Problem (18).

5.1.3. Linear Combination Control Structure for Problem B. The optimal classical control structure is to control y_1 and y_2 with the setpoints −0.427 and 0, respectively, which gives an average profit $J_{av} = 4.750$. Here, we show how this profit can be further increased by selecting a linear combination control structure. In particular, let us consider the control structure wherein the output y_2 is controlled, and a linear combination of the inputs is fixed; that is, $r_1 = y_2$ and $r_2 = a_1u_1 + a_2u_2$. Next, we fix arbitrarily $a_1 = 1$ and find the optimal values of a_2 and the setpoints r_1^{sp} and r_2^{sp} by solving Problem (24). The optimal setpoint values and the corresponding combination matrix Q are given in Table 4. The average profit increases to $J_{av} = 5.056$. Figure 4 shows the operating line and the nominal operating point **d** for this control structure, which requires a single control loop, and increases the profit with respect to point **c**, obtained for the optimal classical control structure.

5.1.4. Conclusions from Case Study 5.1.

Table 4. Selected Linear Combination Control Structure for Problem B

	Q^T					
r	y_1	y_2	y_3	u_1	u_2	$\mathbf{r}^{sp}$
r_1	0	1	0	0	0	0
r_2	0	0	0	1	−1	0.079

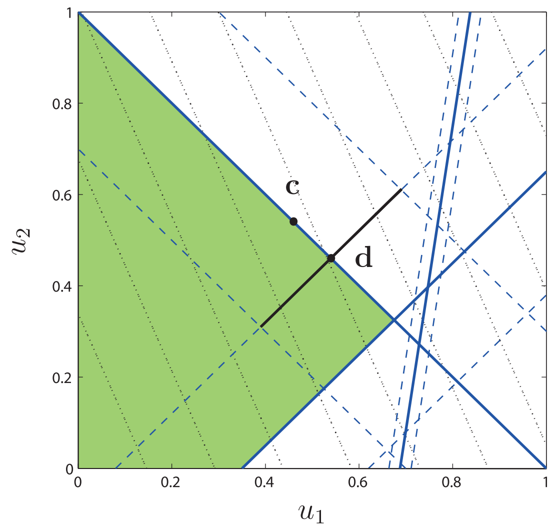

Figure 4. Contour maps for Problem B. Thick black segment: operating line for the control structure in Table 4. Point **c**: nominal operating point for the control structure CS1. Point **d**: nominal operating point for the control structure in Table 4.

- This case study shows a situation for which the steady-state back-off problem with nominal cost is equivalent to the same problem using the average cost. In occurrence, the equivalence holds because we are considering a linear system for which the nominal disturbances are equal to the expected disturbances.
- In Problem A, for which the set of active constraints does not change, the steady-state back-off problems determine that it is optimal to control both active constraints with zero back-off. This corresponds to the well-known constraint control strategy.[45]
- In Problem B, for which the set of active constraints changes with the disturbances, the steady-state back-off problem determines which variables to control and which setpoint values to use. Note that even for a simple linear system this choice is not trivial.
- We have illustrated the importance of computing optimal values for the inputs that are not selected as manipulated variables.
- Finally, we show that it is possible to further increase the operation's economics by selecting a linear combination control structure. Note that, in the SOC literature, linear combination control structures have been used to push the reduced gradient of the cost function to zero.[30,46,47] In this case study, we showed that linear combination control structures may also be useful in cases in which the solution is completely determined by active constraints, and the set of active constraints changes with the disturbance values.

5.2. Continuous Stirred Tank Reactor. Our next case study considers the reactor in the Williams−Otto plant,[48] which consists of an ideal CSTR in which the following reactions take place:

$$A + B \rightarrow C, \quad k_1 = 1.660 \times 10^6 e^{-6666.7/(T_R+273.15)}$$

$$C + B \rightarrow P + E, \quad k_2 = 7.212 \times 10^8 e^{-8333.3/(T_R+273.15)}$$

$$C + P \rightarrow G, \quad k_3 = 2.675 \times 10^{12} e^{-11111/(T_R+273.15)}$$

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The reactants A and B are fed with mass flow rates F_A and F_B, respectively. The desired products are P and E, C is an intermediate product, and G is an undesired product. The reactor is operated isothermally at temperature T_R, with a constant mass holdup of 2105 kg. The dependence of the reaction rate constants k_1, k_2, and k_3 on the absolute temperature is given by Arrhenius' equations. The reader is referred to Marchetti and Zumoffen[34] for the model equations.

For this problem, the input variables are F_B and T_R; that is, $\mathbf{u} = [F_B, T_R]^T$, the measured output variables are the mass fractions of all species, $\mathbf{y} = [X_A, X_B, X_C, X_P, X_G, X_E]^T$, and the sole disturbance is $d = F_A$. The objective is to maximize profit at the steady state subject to input bounds and an upper bound of 0.25 on the mass fraction of B. The optimization problem reads:

$$\begin{aligned} \max_{F_B, T_R} \; & 1200 X_P F + 80 X_E F - 76 F_A - 114 F_B \\ \text{s.t. } & \text{steady-state model equations}, \\ & X_B \le 0.25, \\ & F_B \in [2, 4],\; T_R \in [70, 100]. \end{aligned} \tag{31}$$

where $F = F_A + F_B$. The nominal disturbance value is $F_A = 1.4$ kg/s, and the disturbance range is $F_A \in [1.2, 1.83]$.

In this problem, the constraint on X_B is active at the optimal solution for all disturbance values. The problem has two inputs and one active constraint. The solution is, therefore, not completely determined by the intersection of active constraints. The effect of the disturbance on the optimal solution is depicted in Figure 5. The blue line represents the contour line

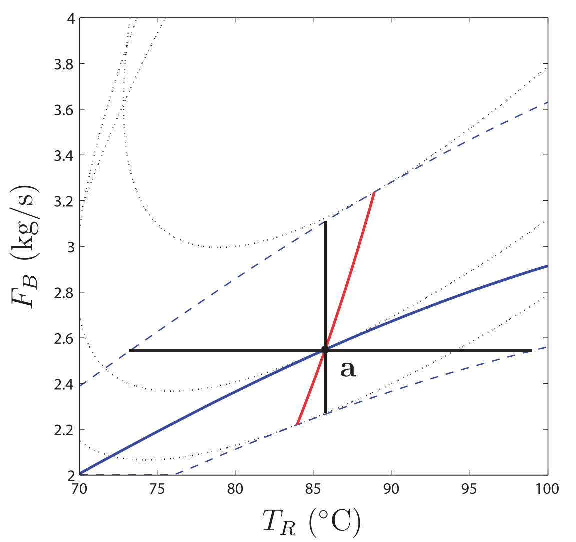

Figure 5. Contour maps for Problem (31). Thick blue line: boundary of the constraint on X_B for the nominal disturbance ($F_A = 1.4$). Blue dashed lines: boundary of the constraint on X_B for the extreme values of the disturbance F_A. Point **a**: nominal optimum. Thick red line: optimal solution map. Dotted lines: contours of the profit. Thick vertical line: operating line for CS4. Thick horizontal line: operating line for CS7.

corresponding to $X_B = 0.25$ at the nominal disturbance, while the lower and upper blue dashed lines show how this contour line moves for the extreme values of the disturbance. Point **a** is the nominal optimum; that is, $\mathbf{a} = \mathbf{u}^*(1.4)$, and the red line represents the optimal solution map $\mathbf{u}^*(F_A)$. In addition, the figure shows the operating lines of the controlled plant using two particular control structures (black vertical line and black horizontal line).

5.2.1. Classical Control Structure for the CSTR. For this problem, there are 28 possible control structures. The seven best control structures are listed in Table 5 according to their optimal value. For each control structure, the nominal and average profit corresponding to the steady-state NLP back-off problems with nominal and average profit maximization is reported as well as the profits obtained using the local disturbance QP approximation of both problems, which is described in section 4.2. In all cases, we use a uniform discretization of the disturbance range $F_A \in [1.2, 1.83]$, with a step of 0.01, which gives $N = 64$ disturbance scenarios. The optimal setpoint values obtained for the average cost NLP back-off problem for each control structure are given in Table 6.

Table 5 was constructed by fixing the control structure in Problem (18) and solving (18) as an NLP.

In the case of the back-off problem with nominal profit, one can see from Table 5 that all the control structures for which the active constraint (the mass fraction X_B) is selected as a controlled variable are optimal solutions that share the same optimal nominal profit. Because we are considering steady-state back-offs (and not dynamic back-offs), and because the set of active constraints does not change for any value of the disturbance, it is optimal in this problem to control the active constraint X_B with zero back-off (i.e., with a setpoint of 0.25). The profit J_n^{NLP} associated with these six control structures corresponds to the profit at the nominal optimum point **a** in Figure 5. Clearly, the back-off problem with nominal profit is not able to differentiate (or rank) these six control structures. Figure 5 also shows the operating lines of the controlled plant using the control structure CS4 (black vertical line) and CS7 (black horizontal line). Note that the operating line of CS4 is closer to the optimal solution line (red line) than that of CS7, and it is clear that for many disturbance values the loss associated with CS7 will be significantly larger than the loss of CS4. Nevertheless, the steady-state back-off problem with nominal profit cannot distinguish between both control structures because it evaluates the profit only at the nominal disturbance value. This shows that the steady-state back-off problem with nominal profit maximization is not useful for selecting a controlled variable for the remaining degree of freedom that is left after controlling the active constraint.

In contrast, the steady-state back-off problem with average profit permits us to correctly rank the control structures according to how well their operating line approximates the optimal solution line. This only requires maximizing the average profit (or minimizing the average cost) instead of the nominal profit (or nominal cost). The unique optimal solution to the steady-state back-off problem with average profit (18) is the control structure CS1, which consists in controlling the active constraint with zero back-off (i.e., the mass fraction X_B with a setpoint of 0.25), and the additional controlled variable X_G with a setpoint of 0.17. The operating line for CS1 is plotted in Figure 6. By controlling X_G, the operating line for CS1 approximates the optimal solution line, which illustrates the self-optimizing behavior of CS1.

5.2.2. Alternatives Solution Strategies. As mentioned in section 3.1.3, the selected solution strategy depends on the complexity of the process model equations. The results obtained for the CSTR problem using different solvers are given in Table 7. The global solver BARON arrived to the optimal CS. However, it experienced difficulties in reducing the cutting

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Table 5. Best CSs for the CSTR Problem[a]

CS	$\mathbf{z}^{O}$						$\mathbf{z}^{I}$					
	X_A	X_B	X_C	X_P	X_G	X_E	F_B	T_R	J_n^{QP} (N = 64)	J_{av}^{QP} (N = 64)	J_n^{NLP} (N = 64)	J_{av}^{NLP} (N = 64)
CS1	0	1	0	0	1	0	0	0	215.79	228.92	215.79	225.16
CS2	0	1	1	0	0	0	0	0	215.79	228.90	215.79	225.15
CS3	1	1	0	0	0	0	0	0	215.79	228.90	215.79	225.04
CS4	0	1	0	0	0	0	0	1	215.79	228.54	215.79	224.88
CS5	0	1	0	0	0	1	0	0	215.79	228.80	215.79	224.78
CS6	0	0	1	0	1	0	0	0	215.15	227.56	212.15	222.50
CS7	0	1	0	0	0	0	1	0	215.79	218.29	215.79	212.26

[a]Ranking based on J_{av}^{NLP}.

Table 6. CSTR Problem: Calculated Setpoints for the Back-off Problem with Average Profit

CS	$\mathbf{r}^{sp}$							
	X_A	X_B	X_C	X_P	X_G	X_E	F_B	T_R
CS1	–	0.250	–	–	0.170	–	–	–
CS2	–	0.250	0.021	–	–	–	–	–
CS3	0.126	0.250	–	–	–	–	–	–
CS4	–	0.250	–	–	–	–	–	86.723
CS5	–	0.250	–	–	–	0.326	–	–
CS6	–	–	0.022	–	0.170	–	–	–
CS7	–	0.250	–	–	–	–	2.561	–

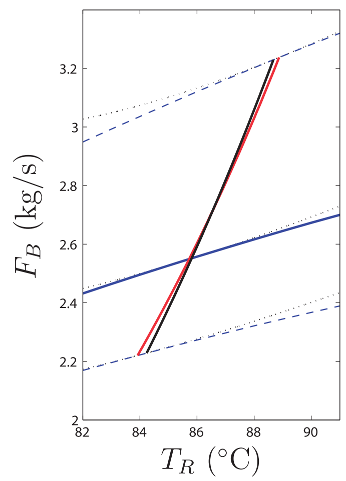

Figure 6. CSTR Problem. Thick black line: operating line for the optimal classical control structure CS1. Thick red line: optimal solution map.

Table 7. CSTR Problem[a]

problem	solver/subsolvers	CS (r)	J_{av}^{NLP}	time (s)
exhaustive search	CONOPT	X_B, X_G	225.158	343.3
MINLP	DICOPT/MINOS, CPLEX	X_B, X_C	225.154	5.2
MINLP	DICOPT/CONOPT, CPLEX	X_B, X_G	225.158	4.1
MINLP	BONMIN/IPOPT, B–B	X_B, X_G	225.158	56.8
MINLP	BARON/BARON, CPLEX	X_B, X_G	225.158	1400(*)
luld-MIQP	CPLEX/CONOPT, CPLEX	X_B, X_G	225.158	0.4

[a]Results obtained using different solvers. Computer used: Intel Core, i5-4440 CPU, 3.10 GHz, 8 GB RAM. Asterisk indicate "interrupted".

criterion gap in acceptable time when the number of disturbance scenarios grows (in this case, up to $N = 64$). Thus, the solver was interrupted when it reached a maximum time without proving convergence to the global optimum. On the other hand, the solvers DICOPT and BONMIN showed good performance, arriving to the optimal CS in an acceptable time. Finally the luld-MIQP approximation converged to the optimal CS, CS1, in only 0.4 s.

5.2.3. Linear Combination Control Structure for the CSTR. Marchetti and Zumoffen[34] showed that the null space method (which is a local SOC method) can be applied to this CSTR problem by controlling the active constrained output X_B and fixing a linear combination of the inputs. The corresponding control structure (taken from Marchetti and Zumoffen)[34] is given in Table 8. The setpoint values are the values of the controlled variables evaluated at the nominal optimum $\mathbf{u}^*(1.4)$. The corresponding operating line in shown in the left plot of Figure 7. One can see that the operating line (black line) is tangent to the optimal solution map (red line) at the nominal optimum point **a**.

Next, we apply the global SOC approach given by the NLP Problem (24). Again, we consider the CS wherein the active constraint X_B is controlled, and a linear combination of the inputs is fixed; that is, $r_1 = X_B$ and $r_2 = aF_B + T_R$. By solving Problem (24), we find the optimal values of the coefficient a and the setpoints r_1^{sp} and r_2^{sp}. The solution is given in Table 8, and the corresponding operating line is shown in the right plot of Figure 7. By comparing both plots, it can be seen how the operating line for the global SOC approach globally approximates the optimal solution map. Nevertheless, the improvement in profit for the global approach is very small because for this particular example, the null space method works very well.

5.2.4. Conclusions from Case Study 5.2.

- This case study clearly shows the limitations of minimizing the nominal cost in back-off approaches. As seen from Table 5 and Figure 5, using the nominal cost does not allow us to distinguish the difference in

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Table 8. Linear Combination CSs for the CSTR Problem

		QT									
	r	X_A	X_B	X_C	X_P	X_G	X_E	F_B	T_R	$\mathbf{r}^{sp}$	J_{av} (N = 64)
global	r_1	0	1	0	0	0	0	0	0	0.250	225.156
SOC	r_2	0	0	0	0	0	0	−0.321	1	0.434	
null	r_1	0	1	0	0	0	0	0	0	0.250	225.155
space	r_2	0	0	0	0	0	0	−0.324	0.946	0.407	

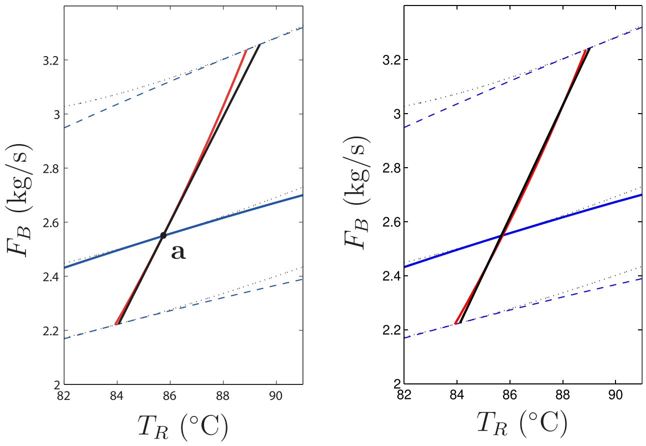

Figure 7. CSTR Problem. Thick red line: optimal solution map. Point **a**: nominal optimum. Thick black lines: operating lines for the linear combination CSs. Left plot: null space method. Right plot: global SOC.

performance between the control structures CS4 and CS7.

- The suitability of the local disturbance MIQP approximation has been illustrated. The proposed luld-MIQP converged to the optimal CS in a reduced time.
- In all cases (MINLP or MIQP approximation with nominal or average cost), the steady-state back-off approach determines that it is optimal to control the active constrained variable X_B with zero back-off (i.e., with a setpoint of 0.25).
- This case study also illustrates that the steady-state back-off problems with average cost minimization are global SOC approaches. The comparison with the null space method illustrates the difference between a global and a local SOC method. For this particular case study, the selected linear combination CSs do not improve (in any significant way) the profit that can be achieved by the best classical CS. The advantage of fixing a linear combination of the inputs in this example might be that a single control loop is required to achieve the optimal profit.

5.3. Evaporator. Our third case study considers the forced-circulation evaporator described by Newell and Lee.[49] The liquid feed mixed with recirculating liquor boils inside the evaporator, which is heated by steam. The generated vapor–liquid mixture is separated in the separator. Most of the separated liquid is recirculated, while a small fraction of it is drawn off as product. The evaporator is illustrated in Figure 8. The main variables are listed in Table 9 together with their nominal values. The model equations can be found in Kariwala et al.[29] The evaporator model has three state variables, L_2, X_2, and P_2, and eight degrees of freedom: the five input variables P_{100}, F_{200}, F_1, F_2, and F_3 and the three disturbances, X_1, T_1, and T_{200}. To stabilize the process, a PI controller is included, which controls the separator level L_2 by manipulating the product flow rate F_2. Therefore, we are going to consider the following variables for the control structure selection problem:

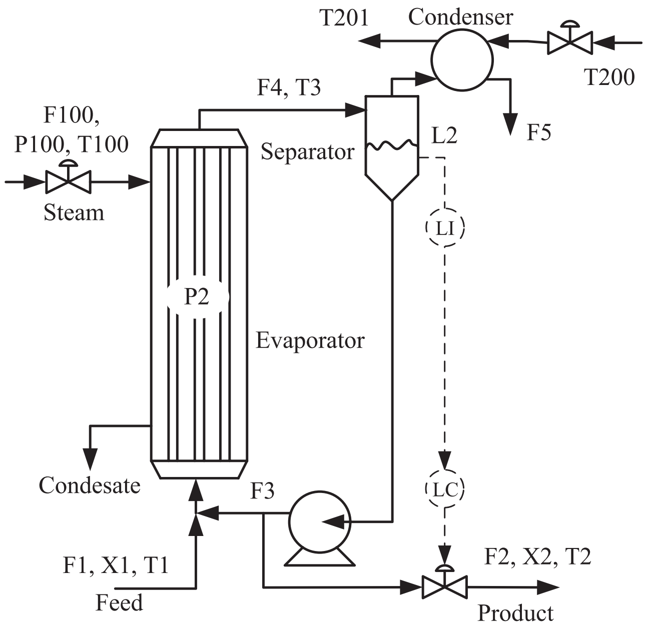

Figure 8. Evaporator system.

Table 9. Evaporator Main Variables and Their Values at the Nominal Optimum

variable	description	value	unit
F_{200}	cooling water flow rate	217.74	kg/min
P_{100}	steam pressure	400.00	kPa
F_3	circulation flow rate	24.72	kg/min
F_1	feed flow rate	9.469	kg/min
X_2	product composition	35.50	%
F_4	vapor flow rate	8.135	kg/min
F_5	condensate flow rate	8.135	kg/min
T_2	product temperature	88.4	°C
T_3	vapor temperature	81.1	°C
P_2	operating pressure	51.41	kPa
F_{100}	steam flow rate	9.434	kg/min
T_{100}	steam temperature	151.5	°C
T_{201}	cooling water outlet temperature	45.55	°C
X_1	feed composition	5.00	%
T_1	feed temperature	40.0	°C
T_{200}	cooling water inlet temperature	25.0	°C
J	profit	582.23	\$/h

$$\mathbf{u} = [F_{200} \quad P_{100} \quad F_3 \quad F_1]^T$$

$$\mathbf{y} = [X_2 \quad F_4 \quad F_5 \quad T_2 \quad T_3 \quad P_2 \quad F_{100} \quad T_{100} \quad T_{201}]^T$$

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Table 10. Optimal CS for the Evaporator

		X_2	F_4	F_5	T_2	T_3	P_2	F_{100}	T_{100}	T_{201}	F_{200}	P_{100}	F_3	F_1
Case A	**z**	1	0	0	0	0	0	0	1	1	0	1	0	0
	$\mathbf{z}^{sp}$	35.5	0	0	0	0	0	0	151.52	46.95	0	400	0	0
Case B	**z**	1	0	0	0	0	0	0	0	0	1	1	1	0
	$\mathbf{z}^{sp}$	35.5	0	0	0	0	0	0	0	0	218.24	400	24.75	0

Table 11. Evaporator Results Using Different Solution Strategies[a]

problem	solver/subsolvers	CS (**r**)	J_{av}	time (s)
exhaustive search	CONOPT	X_2,F_{200},P_{100},F_3	584.89	12 271.1
MINLP	BONMIN/IPOPT,B−B	X_2,F_{200},P_{100},F_3	584.89	3519.1
MINLP	BARON/BARON,CPLEX	X_2,F_{200},P_{100},F_3	584.89	50 000(*)
MINLP	DICOPT/MINOS,CPLEX	X_2,T_{201},P_{100},F_3	581.16	9.8
MINLP	DICOPT/CONOPT,CPLEX	X_2,T_{201},P_{100},F_3	581.16	8.5
lugd-MIQP	CPLEX/CONOPT,CPLEX	X_2,T_{201},P_{100},F_3	581.16	5.6

[a]Computer used: Intel(R) Core(TM), i5-4440 CPU, 3.10 GHz, 8 GB RAM. Asterisks indicate interrupted.

$$\mathbf{d} = [X_1 \quad T_1 \quad T_{200}]^T$$

The nominal values of the disturbance are $X_1 = 5$, $T_1 = 40$, and $T_{200} = 25$, and the disturbance ranges are $X_1 \in [4.75, 5.25]$, $T_1 \in [32, 48]$, and $T_{200} \in [20, 30]$. The objective is to maximize profit at steady state, which is expressed as:

$$J = 4800F_2 - 0.2F_1 - 600F_{100} - 0.6F_{200} - 1.009(F_2 + F_3)$$

where the first term is the value of the product, while the last four terms are operational costs. The optimization problem reads:

$$\begin{aligned} &\max_{\mathbf{u}} J \\ &\text{s.t. steady-state model equations,} \\ &\quad X_2 \geq 35.5 \\ &\quad 40 \leq P_2 \leq 80 \\ &\quad P_{100} \leq 400 \\ &\quad 0 \leq F_{200} \leq 400 \\ &\quad 0 \leq F_1 \leq 20 \\ &\quad 0 \leq F_3 \leq 100 \end{aligned} \tag{32}$$

In this problem, the constraints on X_2 and P_{100} are active for all disturbance scenarios, while the constraint on P_2 may become active at its lower or upper bound depending on the disturbance values.

5.3.1. Classical Control Structure for the Evaporator. The steady-state back-off Problem (18) with average cost minimization will be solved using a grid discretization of the disturbance set $d_{1,k} \in \{4.75\text{: } 0.125\text{: } 5.25\}$, $d_{2,k} \in \{32\text{: } 4\text{: } 48\}$, and $d_{3,k} \in \{20\text{: } 2.5\text{: } 30\}$, which gives a total of $N = 125$ disturbance scenarios. Two cases will be considered. In Case A, Problem (18) is solved without additional constraints, while in Case B, the constraints (21) are included with the RGA bounds $\delta^L = 0.5$ and $\delta^U = 1.5$. The optimal control structure and corresponding setpoint values obtained in both cases are given in Table 10. The problem with Case A is that the controlled variables T_{100} and P_{100} are linearly dependent (see model equations in Kariwala et al.),[29] and therefore, there is a remaining degree of freedom that is used by the MINLP problem to find optimal inputs for each disturbance scenario, which increases the average profit. This, however, cannot be realized by a regulatory feedback control system. This unsuitable CS is avoided in Case B, for which the computation of the RGA matrix requires inverting the controlled subprocess.

As seen in Table 10 for Case B, the optimal CS consists in controlling with zero back-off the constrained variables that are active for all disturbance scenarios. In occurrence, the product composition X_2 is controlled with a setpoint of 35.5, and the input P_{100} is fixed at 400 kPa. In addition, the inputs F_{200} and F_3 are fixed at their computed optimal values.

5.3.2. Alternatives Solution Strategies. The MINLP problem was solved in GAMS using different local and global solvers. The results are showed in Table 11. The local solver DICOPT converged quickly to a feasible suboptimal solution that is quite close to the optimal one. This CS is defined by the controlled outputs are X_2 and T_{201}, the fixed inputs are P_{100} and F_3, and the pairings are X_2−F_1 and T_{201}−F_{200}. On the other hand, the local solver BONMIN, which implements a branch and bound strategy, converged to the optimal CS but in a much higher computational time. The global solver BARON guided us to the optimal solution in around 1896 s, but the computation was interrupted after 50 000 s because it was not possible to close the stopping criterion gap (remaining 29%). The global disturbance MIQP approximation described in section 4.1 was also applied and converged to the same suboptimal solution as the MINLP using DICOPT in a reduced time.

5.3.3. Linear Combination Control Structure for the Evaporator. Next, we find an optimal linear combination control structure by solving the NLP Problem (24) using the same discretization of the disturbance set as in section 5.3.1. Because the constraints on X_2 and P_{100} are active for all disturbance scenarios, we select $r_1 = X_2$ and $r_2 = P_{100}$. The remaining controlled variables r_3 and r_4 will be selected as optimal linear combinations of the variables X_2, F_5, P_2, F_{100}, T_{201}, F_{200}, P_{100}, F_3, and F_1. In addition, the constraint (25) is included with the following matrix T:

$$T = \begin{bmatrix} \left.\dfrac{\partial X_2}{\partial F_{200}}\right|_n & \left.\dfrac{\partial X_2}{\partial P_{100}}\right|_n & \left.\dfrac{\partial X_2}{\partial F_3}\right|_n & \left.\dfrac{\partial X_2}{\partial F_1}\right|_n \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{bmatrix}$$

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Table 12. Optimal Linear Combination CS for the Evaporator

r	Q^T													r^{sp}
	X_2	F_4	F_5	T_2	T_3	P_2	F_{100}	T_{100}	T_{201}	F_{200}	P_{100}	F_3	F_1	
r_1	1	0	0	0	0	0	0	0	0	0	0	0	0	35.5
r_2	0	0	0	0	0	0	0	0	0	0	1	0	0	400
r_3	−57.31	0	1131	0	0	14.13	87.67	0	−38.01	−0.816	1.080	13.38	−1240	−4171
r_4	−9.326	0	172.7	0	0	5.266	17.56	0	−10.94	−0.515	0.044	1.589	−209.6	−1028

As a consequence of selecting $r_1 = X_2$, the first row of T is equal to the first row of the gain matrix G.

It is recommended to solve the NLP problem using different solvers and starting points as one can easily fall in local optima. For this example, the best known solution was found with the solver CONOPT, starting from the nominal optimum. The corresponding combination matrix Q and optimal setpoint values are given in Table 12. The average profit for the $N = 125$ disturbance scenarios is $J_{av} = 609.18$. Recall that the average profit for the best classical control structure was $J_{av} = 584.89$.

5.3.4. Conclusions from Case Study 5.3.

- This case study shows that the steady-state back-off formulation from Problem (18) may lead to a CS that is not steady-state controllable. By selecting controlled variables that are linearly dependent, the controlled process is not invertible, and the values of the manipulated variables are not uniquely determined. These additional degrees of freedom are exploited by the MINLP problem by finding optimal values for the manipulated variables for each disturbance scenario. This, however, cannot be realized by feedback controllers. Although not specifically designed to avoid this problem, the additional constraints of (21) avoid this unsuitable CS as the computation of the RGA matrix requires inverting the controlled subprocess.
- The suitability of the global disturbance MIQP approximation has been illustrated. The lugd-MIQP converged to the same nearly optimal solution found for the MINLP problem using DICOPT.
- The problem of finding a linear combination control structure was illustrated by using a combination matrix Q with a predefined structure and including the constraint (25) with an appropriate choice of matrix T.

6. FINAL CONCLUSIONS

This paper studied steady-state back-off approaches for CS selection based on economics and their link with self-optimizing control. In the literature, back-off approaches typically proceed by minimizing either the nominal cost or the average cost for a given set of disturbance scenarios. A steady-state back-off approach that minimizes the nominal cost is not a SOC approach since it is of little use for selecting controlled variables for the remaining degrees of freedom that are left after controlling all the active constraints.

In contrast, we have shown that the steady-state back-off approach that selects controlled variables and optimal setpoint values by minimizing the average cost is also a SOC approach. Two different formulations of this back-off problem have been studied: (i) the formulation given by the MINLP Problem (18) that selects the optimal classical control structure, and (ii) the formulation given by the NLP Problem (24) that selects an optimal linear combination control structure. Both formulations are global SOC strategies since they are both based on minimizing the average cost in the presence of disturbances. Notice that, the use of linear combination control structures is not a distinctive feature between back-off and SOC methods. It is simply an alternative choice of the controlled variables that allows us to increase the economic performance in many cases.

With respect to the formulation (i), it has been shown that, without additional safeguards, MINLP Problem (18) may lead to unsuitable control structures if the selected controlled variables are linearly dependent. Additional constraints have been added to this formulation to ensure that there exists an input-output pairing that results in an acceptable degree of interaction when decentralized controllers are implemented. The illustrative case studies show that MINLP Problem (18) can be applied regardless of whether or not the set of active constraints changes with the disturbance values. When there are constraints that are active for all disturbance scenarios, the MINLP problem selects to control these active constraints with zero back-offs (which corresponds to the standard constraint control approach) and selects self-optimizing controlled variables for the remaining degrees of freedom. The assumption that the set of active constraints does not change with the disturbance values, which is a standard assumption in local SOC methods, can be viewed as a special case of the back-off approach for which no steady-state back-offs are needed.

On the other hand, the formulation (ii) given by NLP Problem (24) (together with the constraint (25)) represents a general global SOC formulation for selecting optimal linear combinations of output and input variables as CVs, and the corresponding optimal setpoint values. In fact, several recently proposed SOC approaches[36−38] can be viewed as approximations and special cases of NLP Problem (24). In these approaches, the recourse to approximations, such as the use of local loss expressions, responds in part to the attempt to minimize the average loss instead of the average cost. The local and global MIQP approximations were applied to Case Studies 5.2 and 5.3, respectively, showing in both cases their suitability as approximations to the original MINLP formulations.

Based on our findings, we provide the following recommendations for back-off and SOC approaches for CS selection:

- It is recommended to minimize the average cost instead of the nominal cost in back-off approaches. It has been shown that the minimization of the nominal cost may lead to CSs with poor economic performance for disturbance values different from the nominal ones.
- It is recommended to minimize the average cost instead of the average loss in back-off and SOC approaches for CS selection. Evaluating the loss with respect to optimal operation is more involved than evaluating the cost, and it is also unnecessary in view of Remark 1. Once the optimal CS is determined, the associated loss can be evaluated.
- In order to guarantee feasibility for all disturbance scenarios, find optimal setpoint values for all the controlled variables and for all the input variables that are not selected as manipulated variables. Fixing input

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variables at their nominal optimal values may rule out important control structures as infeasible or economically unattractive.

Finally, this paper has focused on steady-state back-off approaches. Dynamic back-off approaches are a different story. However, because dynamic back-off approaches should also pay attention to feasibility and economic performance at steady state, we believe that many of the things we have learned for steady-state back-off approaches can be applied to dynamic back-off approaches as well. For instance, several dynamic back-off approaches fix the inputs that are not selected as manipulated variables at their nominal optimal values, which, as we have seen, may lead to suboptimality or infeasibility issues.

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Notes

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REFERENCES

(1) Luyben, W. L.; Tyréus, B. D.; Luyben, M. L. *Plantwide Process Control*; McGraw-Hill: New York, 1998.

(2) van de Wal, M.; de Jager, A. A review of methods for input/output selection. *Automatica* **2001**, *37*, 487−510.

(3) Skogestad, S.; Postlethwaite, I. *Multivariable Feedback Control. Analysis and Design*, 2nd ed.; John Wiley & Sons: New York, 2005.

(4) Ricardez-Sandoval, L. A.; Budman, H. M.; Douglas, P. L. Integration of design and control for chemical processes: A review of the literature and some new results. *Annual Reviews in Control* **2009**, *33*, 158−171.

(5) Yuan, Z.; Chen, B.; Sin, G.; Gani, R. State-of-the-Art and Progess in the Optimization-based Simultaneous Design and Control for Chemical Processes. *AIChE J.* **2012**, *58*, 1640−1659.

(6) Sharifzadeh, M. Integration of process desing and control: A review. *Chem. Eng. Res. Des.* **2013**, *91*, 2515−2549.

(7) Bahri, P. A.; Bandoni, J. A.; Romagnoli, J. A. Effect of Disturbances in Optimizing Control: Steady-State Open-Loop Backoff Problem. *AIChE J.* **1996**, *42*, 983−994.

(8) Bahri, P. A.; Bandoni, J. A.; Barton, G. W.; Romagnoli, J. A. Back-off calculations in optimizing control: A dynamic approach. *Comput. Chem. Eng.* **1995**, *19* (Suppl), S699−S708.

(9) Figueroa, J. L.; Bahri, P. A.; Bandoni, J. A.; Romagnoli, J. A. Economic Impact of Disturbances and Uncertain Parameters in Chemical Processes − A Dynamic Back-Off Analysis. *Comput. Chem. Eng.* **1996**, *20*, 453−461.

(10) Narraway, L. T.; Perkins, J. D.; Barton, G. W. Interaction between process design and process control: economic analysis of process dynamics. *J. Process Control* **1991**, *1*, 243−250.

(11) Loeblein, C.; Perkins, J. D. Structural Design for On-Line Process Optimization: I. Dynamic Economics of MPC. *AIChE J.* **1999**, *45*, 1018−1029.

(12) Soliman, M.; Swartz, C. L. E.; Baker, R. A mixed-integer formulation for back-off under constrained predictive control. *Comput. Chem. Eng.* **2008**, *32*, 2409−2419.

(13) Narraway, L. T.; Perkins, J. D. Selection of Process Control Structure Based on Linear Dynamic Economics. *Ind. Eng. Chem. Res.* **1993**, *32*, 2681−2692.

(14) Heath, J. A.; Kookos, I. K.; Perkins, J. D. Process Control Structure Selection Based on Economics. *AIChE J.* **2000**, *46*, 1998−2016.

(15) Psaltis, A.; Kookos, I. K.; Kravaris, C. Plant-wide control structure selection methodology based on economics. *Comput. Chem. Eng.* **2013**, *52*, 240−248.

(16) Zumoffen, D. A.; Braccia, L.; Marchetti, A. G. Economic plant-wide control design with backoff estimations using internal model control. *J. Process Control* **2016**, *40*, 93−105.

(17) Kookos, I. K.; Perkins, J. D. Control Structure Selection Based on Economics: Generalization of the Back-Off Methodology. *AIChE J.* **2016**, *62*, 3056−3064.

(18) Kookos, I. K.; Perkins, J. D. An Algorithm for Simultaneous Process Design and Control. *Ind. Eng. Chem. Res.* **2001**, *40*, 4079−4088.

(19) Kookos, I. K.; Perkins, J. D. An algorithmic method for the selection of multivariable process control structures. *J. Process Control* **2002**, *12*, 85−99.

(20) Kookos, I. K. Real-Time Regulatory Control Structure Selection Based on Economics. *Ind. Eng. Chem. Res.* **2005**, *44*, 3993−4000.

(21) Sharifzadeh, M.; Thornhill, N. F. Optimal selection of control structure using a steady-state inversely controlled process model. *Comput. Chem. Eng.* **2012**, *38*, 126−138.

(22) Sharifzadeh, M.; Thornhill, N. F. Integrated design and control using a dynamic inversely controlled process model. *Comput. Chem. Eng.* **2013**, *48*, 121−134.

(23) Mohideen, M. J.; Perkins, J. D.; Pistikopoulos, E. N. Optimal Design of Dynamic Systems under Uncertainty. *AIChE J.* **1996**, *42*, 2251−2272.

(24) Bansal, V.; Perkins, J. D.; Pistikopoulos, E. N. A Case Study in Simultaneous Desing and Control Using Rigorous Mixed-Integer Dynamic Optimization Models. *Ind. Eng. Chem. Res.* **2002**, *41*, 760−778.

(25) Sakizlis, V.; Perkins, J. D.; Pistikopoulos, E. N. Recent advances in optimization-based simultaneous process and control design. *Comput. Chem. Eng.* **2004**, *28*, 2069−2086.

(26) Skogestad, S. Plantwide control: the search for the self-optimizing control structurel. *J. Process Control* **2000**, *10*, 487−507.

(27) Halvorsen, I. J.; Skogestad, S.; Morud, J. C.; Alstad, V. Optimal Selection of Controlled Variables. *Ind. Eng. Chem. Res.* **2003**, *42*, 3273−3284.

(28) Jäschke, J.; Cao, Y.; Kariwala, V. Self-optimizing control - A survey. *Annual Reviews in Control* **2017**, *43*, 199−223.

(29) Kariwala, V.; Cao, Y.; Janardhanan, S. Local Self-Optimizing Control with Average Loss Minimization. *Ind. Eng. Chem. Res.* **2008**, *47*, 1150−1158.

(30) Alstad, V.; Skogestad, S. Null Space Method for Selecting Optimal Measurement Combinations as Controlled Variables. *Ind. Eng. Chem. Res.* **2007**, *46*, 846−853.

(31) Alstad, V.; Skogestad, S.; Hori, E. S. Optimal Measurement Combinations as Controlled Variables. *J. Process Control* **2009**, *19*, 138−148.

(32) Jäschke, J.; Skogestad, S. Optimal operation by controlling the gradients to zero. *Proceedings of the 18th IFAC World Congress*; Milano, Italy, 2011; pp 593−595.

(33) François, G.; Srinivasan, B.; Bonvin, D. Equivalence between neighboring-extremal control and self-optimizing control for steady-state optimization of dynamical systems. *Ind. Eng. Chem. Res.* **2014**, *53*, 7470−7478.

(34) Marchetti, A. G.; Zumoffen, D. A. Self-Optimizing Control Structures with Minimum Number of Process-Dependent Controlled Variables. *Ind. Eng. Chem. Res.* **2014**, *53*, 10177−10193.

(35) Manum, H.; Skogestad, S. Self-optimizing control with active set changes. *J. Process Control* **2012**, *22*, 873−883.

(36) Hu, W.; Umar, L. M.; Xiao, G.; Kariwala, V. Local self-optimizing control of constrained processes. *J. Process Control* **2012**, *22*, 488−493.

(37) Ye, L.; Cao, Y.; Yuan, X. Global Approximation of Self-Optimizing Controlled Variables with Average Loss Minimization. *Ind. Eng. Chem. Res.* **2015**, *54*, 12040−12053.

(38) Ye, L.; Cao, Y.; Skogestad, S. Global Self-Optimizing Control for Uncertain Constrained Process Systems. *IFAC-PapersOnLine* **2017**, *50*, 4672−4677.

(39) Braccia, L.; Marchetti, P. A.; Luppi, P.; Zumoffen, D. Multivariable Control Structure Design Based on Mixed-Integer Quadratic Programming. *Ind. Eng. Chem. Res.* **2017**, *56*, 11228−11244.

DOI: 10.1021/acs.iecr.8b06296
Ind. Eng. Chem. Res. XXXX, XXX, XXX−XXX

(40) Kookos, I. K.; Perkins, J. D. Heuristic-Based Mathematical Programming Framework for Control Structure Selection. *Ind. Eng. Chem. Res.* **2001**, *40*, 2079−2088.
(41) Yelchuru, R.; Skogestad, S. Convex formulations for optimal selection of controlled variables and measurements using Mixed Integer Quadratic Programming. *J. Process Control* **2012**, *22*, 995−1007.
(42) Nocedal, J.; Wright, S. J. *Numerical Optimization*; Springer-Verlag: New York, 1999.
(43) Bazaraa, M. S.; Sherali, H. D.; Shetty, C. M. *Nonlinear Programming: Theory and Algorithms*, 3rd ed.; John Wiley and Sons: Hoboken, NJ, 2006.
(44) Marchetti, A. G.; Ferramosca, A.; González, A. H. Steady-state target optimization designs for integrating real-time optimization and model predictive control. *J. Process Control* **2014**, *24*, 129−145.
(45) Maarleveld, A.; Rijnsdorp, J. E. Constraint control on distillation columns. *Automatica* **1970**, *6*, 51−58.
(46) Cao, Y. Direct and indirect gradient control for static optimization. *International Journal of Automation and Computing* **2005**, *2*, 60−66.
(47) Ye, L.; Cao, Y.; Li, Y.; Song, Z. Approximating Necessary Conditions of Optimality as Controlled Variables. *Ind. Eng. Chem. Res.* **2013**, *52*, 798−808.
(48) Williams, T. J.; Otto, R. E. A generalized chemical processing model for the investigation of computer control. *Trans. Am. Inst. Electr. Eng., Part 1* **1960**, *79*, 458.
(49) Newell, R. B.; Lee, P. L. *Applied Process Control - A Case Study*; Prentice Hall: Englewood Cliffs, NJ, 1989.

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