Null Space Method for Selecting Optimal Measurement Combinations as Controlled Variables

Vidar Alstad[†] and Sigurd Skogestad*

Department of Chemical Engineering, Norwegian University of Science and Technology, Trondheim, Norway

The issue in this paper is to select controlled variables **c** as combinations of the measurements **y**. The objective is to obtain self-optimizing control, which is when we can achieve near-optimal steady-state operation with constant setpoints for the controlled variables, without the need to reoptimize when new disturbances perturb the plant. The null space method yields locally optimal controlled variables $\mathbf{c} = \mathbf{Hy}$ that are linear combinations of measurements **y**. The requirement is that we at least have as many measurements as there are unconstrained degrees of freedom, including disturbances, and that the implementation error is neglected. The method is surprisingly simple. From a steady-state model of the plant, the first step is to obtain the optimal sensitivity matrix **F**, with respect to the disturbances. The optimal matrix **H** satisfies $\mathbf{HF} = 0$; therefore, the next step is to obtain **H** in the left null space of **F**. As an illustration, the method is used to obtain temperature combinations for control of a Petlyuk distillation column.

1. Introduction

For cases with unconstrained control degrees of freedom (inputs u), an important issue is to decide what to control. Although not widely acknowledged by control theorists, controlling the right variables is a key element in overcoming uncertainty in operation.[1,2] This applies also when using advanced control (e.g., model predictive control (MPC)) or real-time optimization (RTO). This paper focuses on the interaction between the local optimization layer and the feedback control layer (see Figure 1), and, more specifically, on the selection of the controlled variables **c** that link these layers. Two subproblems are important here:

(1) *Selection of the controlled variables* **c**. This is a structural decision that is made before the control strategy is implemented.

(2) *Selection of setpoints* $\mathbf{c}_s$. This is a parametric decision that can be done both online and offline.

Here, we focus on the first structural problem of finding the controlled variables and we will assume constant nominal optimal setpoints. As Figure 1 shows, there are two sources of uncertainty that will make a constant setpoint policy nonoptimal: (i) disturbances (d) (these are the external unmeasured disturbances, including parameter variations), and (ii) implementation error (n) (this includes the sum of the effect of the measurement error for **y** and the control error).

Single measurements or functions or combinations of the measurements may be used as controlled variables (**c**). The objective is to obtain self-optimizing control, which is when we can achieve near-optimal steady-state operation with constant setpoints for the controlled variables, without the need to reoptimize when new disturbances perturb the plant. The use of single measurements is simple and is the preferred choice if the loss is sufficiently small. However, for some applications, there may not exist any self-optimizing single measurements, and one may consider measurement combinations. In this paper, we consider linear combinations, that is, $\mathbf{c} = \mathbf{Hy}$, where **H** is a constant matrix.

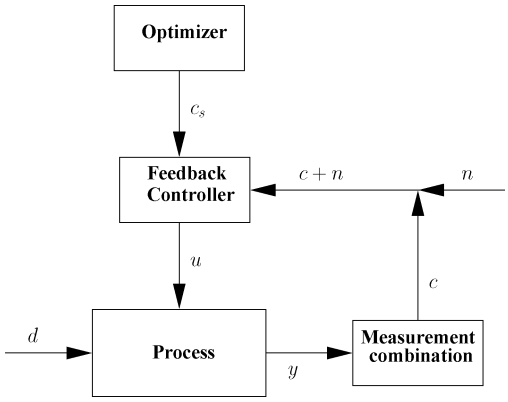

Figure 1. Block diagram of a feedback control structure including an optimizer layer.

Ideas related to self-optimizing control have been presented repeatedly in the process control history, but the first quantitative treatment was that of Morari et al.[1] Skogestad[2] defined the problem more carefully, linked it to previous work, and was the first to include the implementation error as well. He mainly considered the case where single measurements are used as controlled variables; that is, **H** is a selection matrix where each row has a single digit (one, 1) and the rest are zeros (0). The loss with a constant setpoint policy for expected disturbances and implementation errors was evaluated using a "brute-force'' approach. An important advantage of a brute-force evaluation is that one can also identify controlled variables that may yield infeasability for certain disturbances or implementation errors. This was also considered in more detail by Larsson et al.[3] for the Tennessee−Eastman challenge problem and Govatsmark and Skogestad,[4] who suggested adjustment of the setpoints to achieve feasibility. However, the computational load of the "brute-force'' method can be very large, so local methods based on linearizing the behavior around the steady-state are attractive. Skogestad[2] introduced the approximate maximum gain rule as a simple method for selecting controlled variables. In the

* To whom correspondence should be addressed. Tel.: +47 73 59 41 54. Fax: +47 73 59 40 80. E-mail: skoge@chemeng.ntnu.no.

[†] Current affiliation: Norsk Hydro ASA, Oil & Energy Research Center, N-3908 Porsgrunn, Norway.

10.1021/ie060285+ CCC: $37.00 © 2007 American Chemical Society
Published on Web 01/03/2007

multivariable case, the gain is the minimum singular value of the scaled steady-state transfer matrix from **u** to **c**. A similar method was presented by Mahajanam et al.[5] Halvorsen et al.[6] considered the maximum gain method in more detail and also proposed an exact local method that may be used to obtain the optimal measurement combination **H**. However, this method is less attractive computationally and, in addition, is somewhat difficult to use. Hori et al.[7] illustrated the ideas introduced in this paper on indirect control, which can be formulated as a subproblem of the null space method that has been presented in this paper.

Related work has been done by Srinivasan[8−10] on measurement-based optimization to enforce the necessary condition of optimality under uncertainty. The ideas are illustrated on batch processes. Francois et al.[11] extended these ideas and focus on steady-state optimal systems, where a clear distinction is made between enforcing active constraints and requiring the sensitivity of the objective to be zero. Guay and Zhang[12] have presented related ideas on measurement-based dynamic optimization.

In this paper, the objective is to derive a simple method for selecting the optimal measurement combination matrix **H** for the special case with no implementation error. In fact, the method is so simple that the second author (Skogestad) thought it had to be wrong when it was proposed by the first author (Alstad). We have attempted to keep the mathematics as simple as possible. A more-detailed comparison with previous results and extensions are presented in a forthcoming publication (also see ref 13).

2. Problem Formulation

We assume that the operational goal is to use the degrees of freedoms (**u**) to minimize the cost (*J*), while satisfying equality and inequality constraints. The (original) constrained steady-state optimization problem can, for a given disturbance **d**, be formulated as

$$\min_{\mathbf{x},\mathbf{u}} J(\mathbf{x}, \mathbf{u}, \mathbf{d}) \tag{1}$$

subject to

$$\begin{aligned} \mathbf{f}(\mathbf{x}, \mathbf{u}, \mathbf{d}) &= 0 \\ \mathbf{g}(\mathbf{x}, \mathbf{u}, \mathbf{d}) &\le 0 \\ \mathbf{y} &= \mathbf{f}_y(\mathbf{x}, \mathbf{u}, \mathbf{d}) \end{aligned} \tag{2}$$

where $\mathbf{x} \in \mathbb{R}^{n_x}$, $\mathbf{u} \in \mathbb{R}^{n_u}$, and $\mathbf{d} \in \mathbb{R}^{n_d}$ are the states, inputs, and disturbances, respectively; **f** is the set of equality constraints corresponding to the model equation; **g** is the set of inequality constraints that limits the operation (e.g., physical limits on temperature measurements or flow constraints); and **y** represents the measurements.

When solving this optimization problem, we generally find that some constraints are active, corresponding to $g_i(x, u, d) = 0$. To achieve steady-state optimal operation, we assume here that we control all the active constraints[14,15] and that the set of active constraints does not change (see assumption **A3** presented later in this work). Controlling the active constraints consumes a corresponding number of the degrees of freedom (inputs), and we consider, in the following, the remaining *unconstrained* reduced-space optimization problem where the scalar cost function *J* is to be minimized with respect to the n_u remaining degrees of freedom (inputs) **u**:

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

Here, the equality constraints, including the model equations and active constraints, are implicitly included in *J*, so *J* is generally not a simple function of **u** and **d**.

Remark. Although not strictly correct, for simplicity, we use the same symbol for the cost *J* and degrees of freedom **u** in expressions 1 and 3. Also note that it does not matter from a steady-state point of view which of the original degrees of freedom are used to satisfy the active constraints, and which are then left in expression 3 as the unconstrained degrees of freedom **u**, as long as the remaining optimization problem remains well-posed.

We assume that online information about the system behavior is available through measurements **y**. The issue in this paper is finding a set of n_u controlled variables $\mathbf{c} = \mathbf{h}(\mathbf{y})$ associated with the "unconstrained'' degrees of freedom **u**. In the measurement vector **y**, we generally include also the input vector **u**, including the inputs **u′** that have been selected to the control active constraints. However, the measurements of the active constraints are not included in **y**, because they are constant and, thus, provide no information about the operation.

To quantify the difference between alternative control policies, we consider the loss. For a given disturbance *d*, the loss is defined as the difference between the actual cost and the optimal cost.[6]

$$L = J(\mathbf{c}, \mathbf{d}) - J(\mathbf{c}^{\mathbf{opt}}(\mathbf{d}),\mathbf{d}) \approx \frac{1}{2}(\mathbf{c} - \mathbf{c}^{\mathrm{opt}})^{\mathrm{T}}\mathbf{J}_{cc}(\mathbf{c} - \mathbf{c}^{\mathrm{opt}}) \tag{4}$$

where the second-order approximation holds for small deviations from the nominal optimum. The selected controlled variables *c* are assumed to be independent and the Hessian matrix $\mathbf{J}_{cc}$ is assumed to be nonsingular.[6] With a constant setpoint policy, we have $\mathbf{c} = \mathbf{c}_s + \mathbf{n}$, where **n** is the implementation error. In this paper, we assume $\mathbf{n} = 0$ (see assumption **A4** presented later in this work) and assume that the setpoint is nominally optimal, $\mathbf{c}_s = \mathbf{c}^{\mathrm{opt}}(\mathbf{d}^*)$, where $\mathbf{d}^*$ is the nominal value of the disturbance. Then, $\mathbf{c} = \mathbf{c}^{\mathrm{opt}}$ and the loss for small deviations from the nominal optimum is

$$L \approx \frac{1}{2}(\mathbf{c}^{\mathrm{opt}}(\mathbf{d}^*) - \mathbf{c}^{\mathrm{opt}}(\mathbf{d}))^{\mathrm{T}}\mathbf{J}_{cc}(\mathbf{c}^{\mathrm{opt}}(\mathbf{d}^*) - \mathbf{c}^{\mathrm{opt}}(\mathbf{d})) \tag{5}$$

This gives the following insight (which is not very surprising and could have been stated directly): *With independent controlled variables* **c** *and no implementation error, a constant setpoint policy is optimal if* $\mathbf{c}^{\mathrm{opt}}(\mathbf{d})$ *is independent of* **d**, *i.e.* $\mathbf{c}^{\mathrm{opt}}(\mathbf{d}) - \mathbf{c}^{\mathrm{opt}}(\mathbf{d}^*) = 0$.

3. Null Space Method

We consider the unconstrained optimization problem as given by eq 3; that is, we assume "active constraint control", where all optimally constrained variables are assumed to be kept constant at their optimal values. The goal is to find a linear measurement combination $\mathbf{c} = \mathbf{H}\mathbf{y}$ to be kept at constant setpoints $\mathbf{c}_s$. Here, **H** is a constant $n_u \times n_y$ matrix and **y** is a subset of the available measurements. We make the following assumptions:

A1. Steady state: We consider only steady-state operation. The justification for this is that the economics of operation is primarily determined by the steady state. Of course, this assumes that we have a control system in place that can quickly bring the plant to its new steady state.

A2. Disturbances: Only disturbances that affect the steady-state operation are included.

A3. Active constraint control: We assume that the same active constraints remain active for all values of the disturbances and that we control these constraints.

A4. No implementation error: The implementation error is the sum of the control error and the effect of the measurement error. The assumption of no steady-state control error is satisfied if we use a controller with integral action. It is a more serious assumption to neglect the measurement error, so the method implicitly assumes that the measurements have been carefully selected.

We then have the following result.

Theorem 1: Null space method. *Assume that we have n_u independent unconstrained free variables* **u**, *n_d independent disturbances* **d**, *n_y independent measurements* **y**, *and we want to obtain $n_c = n_u$ independent controlled variables* **c** *that are linear combinations of the measurements*

$$\mathbf{c} = \mathbf{H}\mathbf{y} \tag{6}$$

Let

$$\mathbf{F} = \frac{\partial \mathbf{y}^{\mathrm{opt}}}{\partial \mathbf{d}^{\mathrm{T}}}$$

be the optimal sensitivity matrix evaluated with constant active constraints. If $n_y \geq n_u + n_d$, it is possible to select the matrix **H** *in the left null space of* **F**, *$\mathbf{H} \in \mathcal{N}(\mathbf{F}^{\mathrm{T}})$, such that we get*

$$\mathbf{HF} = 0$$

With this choice for **H**, *fixing* **c** *(at its nominal optimal value) is first-order optimal for disturbances* **d***; that is, the loss is zero as long as the sensitivity matrix* **F** *does not change.*

Proof. We first prove that selecting **H** such that $\mathbf{HF} = 0$ gives zero disturbance loss. For small disturbances, the optimal change in the measurements to a change in the disturbances can be written as

$$\mathbf{y}^{\mathrm{opt}}(\mathbf{d}) - \mathbf{y}^{\mathrm{opt}}(\mathbf{d}) = \mathbf{F}(\mathbf{d} - \mathbf{d}^*) \tag{7}$$

where

$$\mathbf{F} = \begin{bmatrix} \dfrac{\partial y_1^{\mathrm{opt}}}{\partial d_1} & \cdots & \dfrac{\partial y_1^{\mathrm{opt}}}{\partial d_{n_d}} \\ & \cdots & \\ \dfrac{\partial y_{n_y}^{\mathrm{opt}}}{\partial d_1} & \cdots & \dfrac{\partial y_{n_y}^{\mathrm{opt}}}{\partial d_{n_d}} \end{bmatrix} \tag{8}$$

is the optimal sensitivity matrix evaluated at the nominal point *. In eq 7, we have only included the first-order term in the Taylor expansion, so eq 7 is valid for small disturbances such that second- and higher-order terms in $(\mathbf{d} - \mathbf{d}^*)$ can be neglected, or, equivalently, as long as *F* does not change. From eq 6, the corresponding optimal change in the controlled variables is $\mathbf{c}^{\mathrm{opt}}(\mathbf{d}) - \mathbf{c}^{\mathrm{opt}}(\mathbf{d}^*) = \mathbf{H}(\mathbf{y}^{\mathrm{opt}}(\mathbf{d}) - \mathbf{y}^{\mathrm{opt}}(\mathbf{d}^*))$ and by inserting eq 7 we get

$$\mathbf{c}^{\mathrm{opt}}(\mathbf{d}) - \mathbf{c}^{\mathrm{opt}}(\mathbf{d}) = \mathbf{HF}(\mathbf{d} - \mathbf{d}^*) \tag{9}$$

From the insight stated at the end of the previous section, the constant setpoint policy is optimal if

$$\mathbf{c}^{\mathrm{opt}}(\mathbf{d}) - \mathbf{c}^{\mathrm{opt}}(\mathbf{d}^*) = 0 \tag{10}$$

which gives the requirement

$$\mathbf{HF}(\mathbf{d} - \mathbf{d}^*) = 0 \tag{11}$$

This must be satisfied for any $(\mathbf{d} - \mathbf{d}^*)$, so we must require that

$$\mathbf{HF} = 0 \tag{12}$$

Next, we must prove the conditions under which this is possible. To satisfy $\mathbf{HF}(\mathbf{d} - \mathbf{d}^*) = 0$, we must select **H** such that $\mathbf{H} \in \mathcal{N}(\mathbf{F}^{\mathrm{T}})$. The rank of the $n_c \times n_y$ matrix **H** is n_u (because $n_y \geq n_c$, $n_c = n_u$, and the controlled variables are independent). The rank of the $n_y \times n_d$ matrix **F** is n_d (because $n_y \geq n_d$ and the disturbances are assumed to be independent). The fundamental theorem of linear algebra says that the left null space of **F** ($\mathcal{N}(\mathbf{F}^{\mathrm{T}})$) has a rank of $n_y - r$, where $r = n_d$ is the rank of **F**. To be able to find an *H* of rank n_u in the left null space of *F*, we must then require $n_y - n_d \geq n_u$ or, equivalently, $n_y \geq n_u + n_d$. □

The proposed null space method is optimal only locally. It is globally optimal in cases where the sensitivity matrix *F* is not dependent on the operating point (disturbances), for example, for a system with a quadratic cost objective and linear model equations (see eq 13, presented later in this work). Nevertheless, based on several case studies, this does not seem to be an important limitation in most practical cases.

Obtaining F. The optimal sensitivity matrix **F** may be computed from the Hessian matrices ($\mathbf{J}_{uu}$ and $\mathbf{J}_{ud}$) and steady-state gain matrices ($\mathbf{G}^y$ and $\mathbf{G}_d^y$), using[6]

$$\mathbf{F} = -(\mathbf{G}^y \mathbf{J}_{uu}^{-1} \mathbf{J}_{ud} - \mathbf{G}_d^y) \tag{13}$$

However, in practice, it is usually easier to obtain **F** directly, by optimizing for the selected disturbances using a nonlinear steady-state model of the plant. Note that we do not necessarily need an explicit representation of the model equations, because we can find **F** numerically. For example, we may use one of the commercial steady-state process simulators, such as Aspen Plus or Hysys. In theory, one may even obtain **F** from experiments on a real operating plant; however, it seems unlikely that this methodology will be sufficiently accurate.

Numerically, the $n_y \times n_d$ matrix **F** may be obtained by perturbing the disturbances **d** and re-solving the optimization problem in eq 3 with the active constraints being constant:

(1) Under nominal conditions ($\mathbf{d} = \mathbf{d}^*$), use the steady-state model to obtain the nominal optimum $\mathbf{y}^{\mathrm{opt}}(d^*)$ and identify the active constraints (finding the nominal optimum may be difficult, because the optimization problem is generally nonconvex).

(2) For each of the n_d disturbances, make a small perturbation ($d_k = d_k^* + \Delta d_k$) and resolve the optimization with the constant active constraints to obtain $\mathbf{y}^{\mathrm{opt}}(d)$ (this is generally simple, because it is only a small perturbation to the existing nominal solution).

(3) Compute $\Delta \mathbf{y}^{\mathrm{opt}} = \mathbf{y}^{\mathrm{opt}}(d) - \mathbf{y}^{\mathrm{opt}}(d^*)$ and obtain **F** numerically using eq 8. A minimum of $n_d + 1$ optimization runs are required; however, more runs may be needed to obtain an accurate estimate for **F**.

Ganesh and Biegler[17] have provided an efficient and rigorous strategy for finding **F**, based on a reduced Hessian method. In addition, some process simulators have built-in optimizers from which the optimal sensitivity **F** may be available.

The next step is to obtain **H**. Numerically, **H** may be obtained from a singular value decomposition of $\mathbf{F}^{\mathrm{T}}$. We have $\mathbf{HF} = 0$ or, equivalently, $\mathbf{F}^{\mathrm{T}}\mathbf{H}^{\mathrm{T}} = 0$. Thus, selecting $\mathbf{H}^{\mathrm{T}}$ as the input

singular vectors of $\mathbf{F}^T$, corresponding to zero singular values in $\mathbf{F}^T$, gives an orthogonal basis.

Example 1. Consider a simple example with one unconstrained degree of freedom u , $n_u = 1$, and one disturbance d, $n_d = 1$. The cost function to be minimized during operation (for varying d) is

$$J(u, d) = (u - d)^2$$

Nominally, $d^* = 0$. We have available two measurements:

$$y_1 = 0.9u + 0.1d$$

and

$$y_2 = 0.5u - d$$

Because $n_y = 2 = n_u + n_d$ and the two measurements are independent, it is possible to find a linear measurement combination

$$\mathbf{c} = \mathbf{H}\mathbf{y} = [h_1 \;\; h_2]\begin{bmatrix} y_1 \\ y_2 \end{bmatrix} = h_1 y_1 + h_2 y_2$$

for which a constant setpoint gives zero disturbance loss, at least locally. We first must obtain the optimal sensitivity matrix **F**. *Optimality is ensured when $(\partial J/\partial u) = 2(u - d) = 0$, which gives $u^{opt} = d$ and $J^{opt} = 0 \; \forall \; d$. The corresponding optimal outputs are*

$$y_1^{opt} = d$$

and

$$y_2^{opt} = -0.5d$$

and (8) gives that $\mathbf{F}^T = [1 \; -0.5]$. Alternatively, use (13) with $\mathbf{G}^{yT} = [0.9 \; 0.5]$, $\mathbf{G}_d^{yT} = [0.1 \; -1]$, $\mathbf{J}_{uu} = 2$, and $\mathbf{J}_{ud} = -2$. From the null space method, the optimal matrix **H** *must satisfy* $\mathbf{HF} = 0$, *or*

$$h_1 f_1 + h_2 f_2 = 0$$

$$h_1 + h_2(-0.5) = 0 \Rightarrow h_1 = 0.5h_2$$

The solution is non-unique. For example, selecting $h_2 = 1$ gives

$$c = 0.5y_1 + y_2$$

Keeping the controlled variable **c** *at its nominally optimal setpoint, $c_s = c^{opt}(d^*) = 0$, gives zero disturbance loss, as is easily verified. Generally, the loss will be zero only locally, i.e., for small changes in d, but, for this example, the cost function is quadratic with linear model equations, and the loss will be zero for any magnitude of the disturbance d.*

4. Discussion

4.1. Measurement Selection. One weakness of the null space method is that it does not consider the measurement error, or, more generally, the implementation error. If we have extra measurements, that is, $n_y > n_u + n_d$, then we have extra degrees of freedom in selecting **H** that should be used to reduce the sensitivity to measurement error. A simple approach is to select a subset of the "best'' measurements such that we get $n_y = n_u + n_d$, but which should these measurements be? This is outside the scope of this paper, and it will be treated in more detail a forthcoming publication on the extended null space method (also see Alstad[13]), but let us provide some results. Let the linear model be

$$\Delta\mathbf{y} = \mathbf{G}^y\Delta\mathbf{u} + \mathbf{G}_d^y\Delta\mathbf{d} = \tilde{\mathbf{G}}^y\begin{bmatrix}\Delta\mathbf{u} \\ \Delta\mathbf{d}\end{bmatrix} \tag{14}$$

where **y** has been scaled, with respect to the expected measurement error, and **u** and **d** have been scaled such that they have similar effects on the cost. It can then be shown that a reasonable approach is to maximize the minimum singular value of the matrix $\tilde{\mathbf{G}}^y = [\mathbf{G}^y\mathbf{G}_d^y]$ from the combined inputs and disturbances to the selected measurements. To understand why this is reasonable, we may imagine using the measurements to backcalculate the inputs and disturbances. For the case with $n_y = n_u + n_d$, $\tilde{\mathbf{G}}^y$ is invertible and we get

$$\begin{bmatrix}\Delta\mathbf{u} \\ \Delta\mathbf{d}\end{bmatrix} = [\tilde{\mathbf{G}}^y]^{-1}\Delta\mathbf{y} \tag{15}$$

To avoid sensitivity to measurement errors in **y**, we want the norm of $[\tilde{\mathbf{G}}^y]^{-1}$ to be small, which is equivalent to wanting a large minimum singular value, $\underline{\sigma}(\tilde{\mathbf{G}}^y)$. From eq 15, we also see why it is reasonable to require $n_y \geq n_u + n_d$ in the null space method, because this is the requirement for being able to uniquely determine all independent variables (inputs and disturbances) from the measurements.

4.2. Freedom in Selecting H. Even for the case $n_y = n_u + n_d$, there are an infinite number of matrices **H** that satisfy $\mathbf{HF} = 0$. This stems from the freedom of selecting basis vectors for the null space. Let $\mathbf{H}_0$ be one such matrix, i.e., $\mathbf{H}_0\mathbf{F} = 0$. For example, $\mathbf{H}_0$ may consist of the one set of basis vectors that span the null space of $\mathbf{F}^T$. Then, $\mathbf{H} = \mathbf{C}\mathbf{H}_0$ also satisfies $\mathbf{HF} = 0$, provided the $n_c \times n_c$ matrix **C** is nonsingular.

Actually, the degrees of freedom in selecting **C** (and **H**) are the same as the degrees of freedom that are used in steady-state decoupling (or similar) in control. The linear model for the selected controlled variables can be written as

$$\Delta\mathbf{c} = \mathbf{H}\Delta\mathbf{y} = \mathbf{H}\mathbf{G}^y\Delta\mathbf{u} + \mathbf{H}\mathbf{G}_d^y\Delta\mathbf{d} = \mathbf{G}\Delta\mathbf{u} + \mathbf{G}_d\Delta\mathbf{d} \tag{16}$$

and the degrees of freedom in the matrix **C** may be used to affect $\mathbf{G} = \mathbf{H}\mathbf{G}^y$ and $\mathbf{G}_d = \mathbf{H}\mathbf{G}_d^y$. For example, it is possible to select **H** such that $\mathbf{G} = \mathbf{I}$, and we have a decoupled steady-state response from **u** to **c**.

4.3. Disturbances. The minimum number of measurements required in the null space method ($n_u + n_d$) may be large if we have many disturbances (a large n_d value). Therefore, in practical applications, it is desirable to reduce the number of disturbances. Unfortunately, there does not seem to be any simple rigorous procedure for eliminating unimportant disturbances, although some approaches are discussed in Chapter 5 of the work by Alstad.[13] It is obvious that we may eliminate disturbances d_i that satisfy both of the following conditions: (1) no steady-state effect on the measurements (**y** is independent of d_i, i.e., $\mathbf{G}_{d_i}^y = $), and (2) no steady-state effect on the optimal operation ($\mathbf{u}^{opt}$ is independent of d_i).

It could be argued that we may eliminate all "unobservable'' disturbances that satisfy condition 1, because we have no way of detecting them and, thus, correcting for them. However, such disturbances may affect the optimal operation and result in large losses; therefore, an analysis based on neglecting them may be highly misleading. To achieve acceptable operation in such cases, we must obtain additional measurements, for example, of the disturbance itself. One example would be a price change, as is discussed in more detail below. Also, we cannot eliminate

all disturbances that have no effect on optimal operation and thus satisfy condition 2. This is because the disturbance may effect a measurement, and controlling this measurement will then result in a loss.

In practice, with too few measurements, one may eliminate some disturbances and obtain the controlled variables $\mathbf{c} = \mathbf{Hy}$ using the null space method, but, afterward, one should analyze the loss with all disturbances included. Alternatively, one may be able to obtain the optimal combination numerically using the exact local method of Halvorsen et al.[6] or the extended null space method that will be presented in a forthcoming publication.

4.4. Physical Interpretation. The proposed null space method yields controlled variables that are linear combinations of the available measurements. A disadvantage is that the physical interpretation of what we control is usually lost. This is by no means a fundamental limitation, because, in principle, we can control any signal from the process, as long as it is independent. Thus, if all measurements are regarded as signals, the concept of controlling a combination of signals may be easier to grasp. If possible, one can choose to combine measurements of one type, for instance, only temperatures (e.g., in a distillation column) or only mass flows. In any case, we can scale variables such that the resulting measurements are dimensionless, which is common in practice.

4.4.1. Change in Active Constraints. It has been assumed that the set of active constraints does not change. If they may change, then one must, for each set of active constraints, obtain new controlled variables $\mathbf{c} = \mathbf{Hy}$ satisfying $\mathbf{HF} = \mathbf{0}$, where $\mathbf{F}$ is evaluated with the given set of active constraints. This involves offline calculations. In addition, one must have an online strategy for identifying a change in active constraints change and some logic for switching to a new set of controlled variables. Thus, for cases where the active constraints shift frequently with the disturbances, other online methods may be better suited, for example, real-time optimization (RTO) combined with model predictive control (MPC). Alternatively, we could use the ideas of Arkun and Stephanopoulos[15] in regard to how to handle varying active constraints.

4.5. Nonobservable Disturbances and Price Changes. Self-optimizing control is based on using feedback to detect disturbances and optimally adjust the inputs to achieve near-optimal operation. Thus, one must require that the disturbances are observable (visible) in the measurements $\mathbf{y}$. One example of a "disturbance'' that is not visible in the measurements is prices. However, prices (p_i) do enter in the objective function, because typically $J = \sum_i p_i x_i$, and price changes will change the optimal point of operation.

To handle price changes (or, more generally, disturbances that are not observable in the measurements $\mathbf{y}$), one must assume that the price (disturbances) is known (measured). Price changes can then be handled in two ways:

(1) Adjust the setpoints in a feedforward manner. Then, for a price change $\Delta\mathbf{p}$, we have that

$$\mathbf{c}_s = \mathbf{c}_s(p^*) + \mathbf{HF}_p\Delta\mathbf{p} \tag{17}$$

where $\mathbf{F}_p = (\partial\mathbf{y}^{opt}/\partial\mathbf{p}^T)$ is the optimal sensitivity from the prices to the measurements.

(2) Include the prices as extra measurements in y and use the regular procedure of selecting self-optimizing control variables, as previously described.

The first approach is probably the simplest and most transparent.[18]

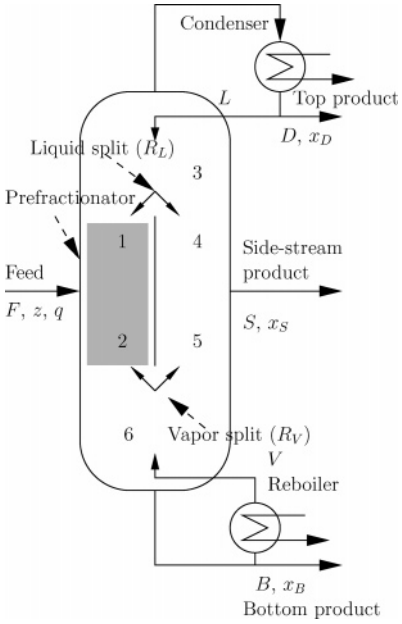

Figure 2. Schematic of the Petlyuk distillation column implemented in a single shell ("divided wall column").

4.6. Limitations. As already mentioned, the proposed null space method is optimal only locally. It is globally optimal in cases where the sensitivity matrix $\mathbf{F}$ is not dependent on the operating point. Nevertheless, based on several case studies, this does not seem to be an important limitation in most practical cases. Other possibly more-serious limitations for practical use are that (1) implementation errors are not explicitly handled (except through the selection of which measurements to use), (2) the active constraints are assumed not to change (as discussed previously, in more detail), (3) the optimal setpoint for c must be obtained (not really a limitation, but rather a fact), and (4) the derivation of the optimal measurement combination $\mathbf{c} = \mathbf{Hy}$ is based on steady-state models, and one must later check that the resulting structure has acceptable dynamic controllability (this may usually be achieved using a cascade control structure where local controllers handle the dynamic response and c is controlled at steady state using the setpoints for the local controllers as manipulated variables).

5. Petlyuk Distillation Case Study

5.1. Introduction. The Petlyuk distillation column is an appealing alternative for the separation of ternary mixtures. Compared with the traditional configuration of two columns in series, typical savings on the order of 30% are reported in *both* energy and capital costs.[19] However, the savings in energy may be difficult to achieve in practice, and the goal here is to suggest simple control policies. We are looking for a "self-optimizing" control structure that, despite external disturbances and measurements errors, gives near-optimal operation with constant setpoints.

The Petlyuk column has six sections and may be implemented as a "divided wall'' column, as illustrated in Figure 2. The boilup and reflux streams are split at the dividing wall with split fractions $R_V = V_2/V_6$ and $R_L = L_1/L_3$, respectively. With a given feed and pressure, the Petlyuk column has five steady-state degrees of freedom. For example, these may be selected as

$$\mathbf{u}_{all}^T = [L \;\; V \;\; S \;\; R_L \;\; R_V] \tag{18}$$

Table 1. Data for Petlyuk Case Study

parameter	value
Column Data	
number of stages in each section	$N_T = 8$
relative volatilities	$\alpha^T = [9\ 3\ 1]$
boiling point A, B, and C [K]	$\mathbf{T}_B^T = [299.3\ 342.15\ 399.3]$
Feed	
flow	$F^* = 1$
composition	$\mathbf{z}^{*T} = [1/3\ 1/3\ 1/3]$
liquid fraction	$q^* = 0.477$
Product Compositions	
distillate	$x_{A,D}^0{}^* = 0.97$
side-stream	$x_{B,S}^0{}^* = 0.97$
bottom	$x_{C,B}^0{}^* = 0.97$
Disturbances (d)	
feed flow	$F = F^* \pm 0.1$
feed composition	
z_A	$z_A = z_A^* \pm 0.1$
z_B	$z_B = z_B^* \pm 0.1$
liquid fraction	$q = q^* \pm 0.1$
product specification	
$x_{A,D}^0$	$x_{A,D}^0 = x_{A,D}^0{}^* \pm 0.01$
$x_{C,B}^0$	$x_{C,B}^0 = x_{C,B}^0{}^* \pm 0.01$
$x_{B,S}^0$	$x_{B,S}^0 = x_{B,S}^0{}^* \pm 0.01$
Measurement/Implementation Errors (n)	
temperatures	0.5 K (absolute)
flows	2.5% (relative)
R_L, R_V	0.025 absolute

corresponding to the reflux, boilup, side-stream flow, liquid split, and vapor split, respectively.

Assume that the feed consists of three key components A, B, and C, with mole fractions $\mathbf{z}^T = [z_A\ z_B\ z_C]$, a molar flow rate F, and a liquid fraction q. The light component A dominates in the distillate stream (D) and component B dominates in the side-stream (S), whereas the heavy component C dominates in the bottom stream (B).

We consider a case study with a relative volatility of 3 between the key components and eight theoretical stages in each of the six sections. Key data are given in Table 1, and further details are found in Chapter 8 in the work by Alstad.[13]

We assume that the operational objective is to use the five degrees of freedom to minimize the energy usage, $J = V$, while maintaining the following three product specifications ("active constraints''): (1) distillate purity ($x_{A,D}$), (2) bottom purity ($x_{C,B}$), and (3) side-stream purity ($x_{B,S}$), where $x_{i,j}$ is the mole fraction of component i in stream j. Minimizing the energy (V), with respect to the remaining two degrees of freedom, gives an unconstrained nominal optimum, with

$$\mathbf{u}_{\text{all}}^{\text{opt}}(\mathbf{d}^*)^T = [L^*\ \ V^*\ \ S^*\ \ R_L^*\ \ R_V^*] = [0.7618\ \ 0.5811\ \ 0.3227\ \ 0.3792\ \ 0.5123]$$

The minimum boilup ($V_{\min}$) with an infinite number of stages is $V_{\min}^{\infty} = 0.5438$; therefore, the nominal optimal boilup of 0.5811 is ~6% higher than the theoretical minimum.

Because the objective is to minimize the boilup, which also is an input, one may mistakenly believe that one can use an open-loop approach, where the optimal value for the boilup is calculated and implemented in the column, $V = V^{\text{opt}}$. However, Halvorsen and Skogestad[20] noted that such an approach is impossible (or at least very difficult):

(1) The operation is infeasible for $V < V^{\text{opt}}$, so we must ensure that $V \geq V^{\text{opt}}$.

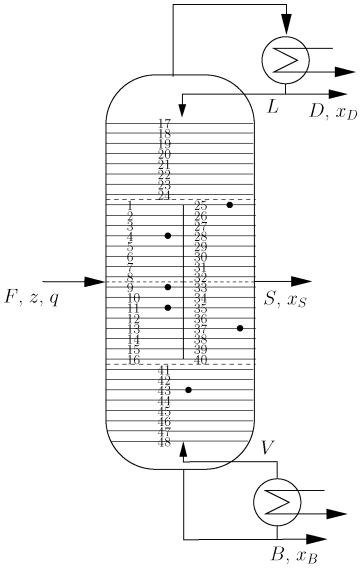

Figure 3. Physical location of the best subset of measurements for alternative 1.

Table 2. Alternative Control Structures

Alternative	c_1	c_2	c_3	c_4	c_5	
1	$x_{A,D}$	$x_{B,S}$	$x_{C,B}$	c_{tdf}^1	c_{tdf}^2	null space method, use R_V and R_L
2	$x_{A,D}$	$x_{B,S}$	$x_{C,B}$	R_V	c_{odf}	null space method, fix R_V
3	$x_{A,D}$	$x_{B,S}$	$x_{C,B}$	R_V	DT_S	fix DT_S and R_V
4	$x_{A,D}$	$x_{B,S}$	$x_{C,B}$	R_V	R_L	constant splits R_V and R_L

(2) The optimal value of V varies, with respect to the disturbances, and may be difficult to find, requiring a detailed model and a direct measurement of the disturbances (or a very accurate estimate) to be viable. This is unrealistic in most cases.

(3) The measurement or estimation of V may be difficult to achieve (measuring vapor flow); thus, it may be sensitive to measurement error when trying to implement the optimal V.

Thus, the approach here is to use self-optimizing control. As candidate measurements ($\mathbf{y}$), we include all flows (ratioed to the feed), as well as the temperature at all stages. This gives ~60 measurements. The component compositions in each product stream are also measured; however, because of the fact that they are active constraints (and, thus, are constant), they are not useful for self-optimizing control and are not included in $\mathbf{y}$.

Alternative 1: Two Degrees of Freedom. We first consider using the two available unconstrained degrees of freedom ($n_u = 2$) to control (and fix) two measurement combinations. The two unconstrained degrees of freedom could, for example, be $u = [R_L\ R_V]$ (but the specific choice does not actually matter for the steady-state analysis). The assumed disturbance vector is (these are determined to be the most important disturbances, from those listed in Table 1)

$$\mathbf{d}_{\text{tdf}} = \begin{bmatrix} z_A \\ z_B \\ q \\ x_{B,S} \end{bmatrix} \tag{19}$$

where the subscript "tdf" denotes that the are two degrees of freedom. The last entry represents the composition offset for the side-stream product. The feed rate F is not included, because we have chosen to use only intensive variables when forming

Table 3. Percentage Loss (in *V*) for All Disturbances[a]

	Loss [%]							
Alternative	F_-	F_+	z_{A-}	z_{A+}	z_B-	z_{B+}	q_-	$q+$
1	0.0	0.0	0.0171	0.0207	0.0166	0.0111	0.0001	0.0000
2	0.0	0.0	0.0037	0.1340	0.2247	0.1666	0.1876	0.1084
3	0.0	0.0	5.0840	11.8810	0.3469	0.8295	1.0441	1.1740
4	0.0	0.0	46.7037	6.3019	95.1660	9.8256	32.4629	6.0578

	Loss [%]							
Alternative	x^0_{A,D_+}	x^0_{A,D_-}	x^0_{C,B_+}	x^0_{C,B_-}	x^0_{B,S_+}	x^0_{B,S_-}	$(L_n^{max})^b$	$(L_n^{avg})^c$
1	0.0025	0.0095	0.0639	0.2082	0.0002	0.0007	0.0213	0.0117
2	0.0040	0.0110	0.0060	0.0174	0.0004	0.0004	0.0847	0.0206
3	0.0074	0.0207	0.0033	0.0034	0.0025	0.0075	0.2108	0.0475
4	0.0262	0.0253	0.0245	0.0311	0.2579	1.0198	9.3142	3.6254

[a] The symbol "−'' in the subscript denotes negative perturbation, whereas "+'' in the subscript denotes positive perturbation from the nominal value. [b] Maximum loss for the implementation errors. [c] Average loss for the implementation errors.

the controlled variables (with a constant column efficiency, a feed rate change is automatically compensated for at steady state by fixing intensive variables).

To use the null space method, we need from Theorem 1 to combine $n_u + n_d = 2 + 4 = 6$ measurements. To select the best subset of 6 out of the ~60 candidate measurements, we use the measurement selection approach mentioned in the discussion section. This results in the following six temperature measurements:

$$\mathbf{y}_{\text{tdf}} = \begin{bmatrix} T_{37} \\ T_{11} \\ T_{43} \\ T_{25} \\ T_4 \\ T_9 \end{bmatrix} \tag{20}$$

The location of the selected measurements is shown in Figure 3. Note that the majority of measurements are located in the bottom portion of the column, whereas only two measurements are located above the feed point. The sensitivity matrix **F** was obtained numerically by perturbing each of the four disturbances and reoptimizing. The null space method in Theorem 1 gives the optimal matrix **H**, corresponding to the following measurement combinations (controlled variables):

$$c_{\text{tdf},1} = -0.472T_{37} + 0.312T_{11} + 0.113T_{43} - 0.457T_{25} + 0.561T_4 - 0.378T_9 \tag{21}$$

$$c_{\text{tdf},2} = 0.185T_{37} + 0.376T_{11} - 0.667T_{43} - 0.524T_{25} - 0.154T_4 + 0.285T_9 \tag{22}$$

Alternative 2: One Degree of Freedom. Until now, we have assumed that the vapor split R_V is a degree of freedom during operation (available for manipulation); however, most likely, this is not possible in practice. Therefore, it is interesting to consider the case where R_V is fixed. In fixing R_V , we add the implementation error of controlling R_V to the disturbance vector and get

$$\mathbf{d}_{\text{odf}} = \begin{bmatrix} z_A \\ z_B \\ q \\ x_{B,S} \\ R_V \end{bmatrix} \tag{23}$$

The corresponding minimum number of measurements needed for the null space method is $n_u + n_d = 1 + 5 = 6$. The following subset of measurements was obtained:

$$\mathbf{y}_{\text{odf}} = \begin{bmatrix} T_{37} \\ T_{10} \\ T_{43} \\ T_{27} \\ T_5 \\ T_{12} \end{bmatrix} \tag{24}$$

which is very similar to the two-degrees-of-freedom case. The optimal measurement combination from the null space method is

$$c_{\text{odf}} = -0.388T_{37} - 0.658T_{10} + 0.192T_{43} - 0.0471T_{27} + 0.448T_5 + 0.421T_{12} \tag{25}$$

Loss Evaluation Using a Nonlinear Model. The two previously mentioned control structures are compared with two alternative control structures (see Table 2). Alternative 3 is a control structure proposed by Halvorsen and Skogestad,[20] where $c_{DTS} = (T_4 - T_{28}) + (T_{12} - T_{36})$ is a symmetry measure of the temperature difference over the dividing wall, whereas alternative 4 is the "open loop" approach.

The nonlinear losses for the alternative control structures for different realistic magnitude of the disturbances and measurement errors are given in Table 3. In the table, we have also included losses for changes ("disturbances'') in the distillate and bottom product compositions (active constraints), which were not included in the original disturbances used to derive c_{tdf} and c_{odf}.The conclusion is that the self-optimizing properties are excellent for both alternatives 1 and 2. When fixing two measurement combinations in alternative 1, the loss in energy usage (V) is <0.02% for the disturbances considered and ≳0.2% for a disturbance in the bottom composition (which was not considered when deriving c_{tdf}). The losses, with respect to implementation errors, are also very small. When fixing R_V and c_{odf} (alternative 2), the loss is ~10 times higher for the previously considered disturbances; however, it is still only ~0.2% and, thus, is insignificant, from a practical point of view. Because the loss is so small, the strategy of fixing R_V and c_{odf} is clearly preferred for practical implementations. The losses for the other two control structures are higher, with a maximum disturbance loss of 11% for alternative 3 and 95% for alternative 4. Alstad[13] also considered alternatives where R_V and a single

temperature was fixed. The best methodology was to fix a temperature just below the side stream with a maximum disturbance loss of ~1.4%.

In the work of Alstad,[13] nonlinear closed-loop dynamic simulations are shown, which confirm the practical implementation of alternative 2.

6. Conclusion

This paper has introduced the null space method for selecting controlled variables **c**. We consider a constant setpoint policy, where the controlled variables are kept at constant setpoints $\mathbf{c}_s$. We propose to select self-optimizing controlled variables as linear combinations $\mathbf{c} = \mathbf{H}\mathbf{y}$ of a subset of the available measurements **y**. With no implementation error, it is locally optimal to select **H** such that $\mathbf{HF} = 0$, where $\mathbf{F} = (\partial \mathbf{y}^{opt}/\partial \mathbf{d}^T)$ is the optimal sensitivity, with respect to disturbance **d**. However, ignoring the implementation error is a serious shortcoming for some applications. To compensate for this partially, it is important to use measurements **y** that are independent and not sensitive to measurement error. Another shortcoming is that a new set of controlled variables (for the unconstrained degrees of freedom) must be found for each possible set of active constraints. The global properties of the proposed variable combination $\mathbf{c} = \mathbf{H}\mathbf{y}$ must be evaluated by computing the loss for expected disturbances and implementation errors using the nonlinear model, and a controllability analysis should also be performed before implementation. The method has been illustrated on a Petlyuk distillation example, where we find that the null space method yields controlled variables with very small losses.

Literature Cited

(1) Morari, M.; Stephanopoulos, G.; Arkun, Y. Studies in the synthesis of control structures for chemical processes. Part I: Formulation of the problem, process decomposition and the classification of the controller task. Analysis of the optimizing control structures. *AIChE J.* **1980**, *26* (2), 220−232.

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

(3) Larsson, T.; Hestetun, K.; Hovland, E.; Skogestad, S. Self-Optimizing Control of a Large-Scale Plant: The Tennessee Eastman Process. *Ind. Eng. Chem. Res.* **2001**, *40* (22), 4889−4901.

(4) Govatsmark, M. S.; Skogestad, S. Selection of controlled variables and robust setpoints. *Ind. Eng. Chem. Res.* **2005**, *44* (7), 2207−2217.

(5) Mahajanam, R.; Zheng, A.; Douglas, J. A shortcut method for controlled variable selection and its application to the butane alkylation process. *Ind. Eng. Chem. Res.* **2001**, *40* (14), 3208−3216.

(6) Halvorsen, I. J.; Skogestad, S.; Morud, J. C.; Alstad, V. Optimal selection of controlled variables. *Ind. Eng. Chem. Res.* **2003**, *42* (14), 3273−3284.

(7) Hori, E. S.; Skogestad, S.; Alstad, V. Perfect steady-state indirect control. *Ind. Eng. Chem. Res.* **2005**, *44* (4), 863−867.

(8) Srinivasan, B.; Primus, C. J.; Bonvin, D.; et al. Run-to-run optimization via control of generalized constraints. *Control Eng. Pract.* **2001**, *9* (8), 911−919.

(9) Srinivasan, B.; Bonvin, D.; Visser, E. Dynamic optimization of batch processes—I. Characterization of the nominal solution. *Comput. Chem. Eng.* **2003**, *27* (1), 1−26.

(10) Srinivasan, B.; Bonvin, D.; Visser, E.; et al. Dynamic optimization of batch processes—II. Role of measurements in handling uncertainty. *Comput. Chem. Eng.* **2003**, *27* (1), 27−44.

(11) Francois, G.; Srinivasan, B.; Bonvin, D. Use of measurements for enforcing the necessary conditions of optimality in the presence of constraints and uncertainty. *J. Process Control* **2005**, *15* (6), 701−712.

(12) Guay, M.; Zhang, T. Adaptive extremum seeking control of nonlinear dynamic systems with parametric uncertainties. *Automatica* **2003**, *39* (7), 1283−1293.

(13) Alstad, V. Studies on the Selection of Controlled Variables, Ph.D. Thesis, Norwegian University of Science and Technology, 2005. Available via the Internet at the home page of S. Skogestad: http://www.nt.ntnu.no/users/skoge/publications/thesis/2005_alstad/.

(14) Maarleveld, A.; Rijnsdorp, J. E. Constraint control on distillation columns. *Automatica* **1970**, *6* (1), 51−58.

(15) Arkun, Y.; Stephanopoulos, G. Studies in the Synthesis of Control Structures for Chemical Processes: Part IV. Design of Steady-State Optimizing Control Structures for Chemical Process Units. *AIChE J.* **1980**, *26* (6), 975−991.

(16) Strang, G. *Linear Algebra and Its Applications*, 3rd Edition; Harcourt Brace & Company: 1988.

(17) Ganesh, N.; Biegler, L. T. A reduced Hessian strategy for sensitivity analysis of optimal flow sheets. *AIChE J.* **1987**, *33* (2), 282−296.

(18) Skogestad, S. Near-optimal operation by self-optimizing control: From process control to marathon running and business systems. *Comput. Chem. Eng.* **2004**, *29* (1), 127−137.

(19) Triantafyllou, C.; Smith, R. The design and operation of fully thermally coupled distillaton columns. *Trans. Inst. Chem. Eng.* **1992**, *7* (A), 118−132.

(20) Halvorsen, I. J.; Skogestad, S. Optimal operation of Petlyuk distillation: Steady-state behavior. *J. Process Control* **1999**, *9*, 407−424.

Received for review March 9, 2006
Revised manuscript received November 9, 2006
Accepted November 10, 2006

IE060285+