# Process Control Structure Selection Based on Economics

**Jonathan A. Heath, Ioannis K. Kookos, and John D. Perkins**
Centre for Process Systems Engineering, Dept. of Chemical Engineering and Chemical Technology,
Imperial College of Science, Technology and Medicine, London SW7 2BY, U.K.

*In process systems, selecting suitable sets of manipulated and controlled variables and the design of their interconnection, known as the control structure selection problem, is an important structural optimization problem. The operating performance of a plant depends on the control structure selected, as well as the characteristics of the disturbances acting on the plant. The economic penalty associated with the variability of main process variables close to active constraints was used in this work to develop a quantitative measure for the ranking of alternative control structures. The problem is formulated as a mixed integer nonlinear optimization problem of special structure, which was used for an algorithm to solve this problem to global optimality. The final formulation is a mixed integer linear problem for which effective solution methods are currently available. The validity and usefulness of the method are demonstrated through a number of case studies.*

## Introduction

An important structural decision in terms of the operating performance of a process plant is related to the selection of suitable sets of manipulated and controlled variables, and the design of their interconnection. This problem is known as the control structure selection problem. The last two decades have witnessed important theoretical developments in this area, and two major approaches have emerged. The first approach is based on qualitative methods. Heuristic and logical rules are used in sequential decisions that lead to the invention of feasible and plausible control structures. The work of Buckley (1964) had a profound impact on the development of these methods. Most of the available literature is reviewed in Stephanopoulos (1983) and in Luyben et al. (1999). The second approach uses quantitative methods where mathematical models are formulated and solved using mathematical programming methods. Georgiou and Floudas (1989), Moore (1992), Luyben and Floudas (1992), Turkay et al. (1993), Narraway and Perkins (1993, 1994), and Mohideen et al. (1996) have presented methodologies that fall into this category. The main advantage of the heuristic-based approaches stems from the fact that they do not involve any detailed evaluation. As a result, the engineering effort and computational time can be negligible even for large-scale problems. The mathematical programming-based methods, on the other hand, are rigorous and produce structures that are optimal within the limitations imposed by the mathematical methods and models used. An obvious limiting factor in the latter approaches is the size and complexity of the models that can be tackled within a mathematical programming framework. The method presented in this article belongs to the mathematical programming-based methods and, as such, it consists of three major elements (Nishida et al., 1981; Morari and Perkins, 1995): *the problem representation, the problem evaluation, and the solution strategy.* The rationale behind the elements employed in this work is briefly discussed in what follows.

Nishida et al. (1981) state that the main task of chemical process control synthesis is to structure a dynamic system of measurements and manipulated variables so that certain control objectives are satisfied in the presence of disturbances. They divide these control objectives into two main categories. The first set of control objectives stems from purely economic considerations and can be related to the optimization of an objective function that accounts for the profitability of the plant. These control objectives are assigned to the (steady-state) optimizing control system. The second set of control objectives is related to maintaining certain process variables within the constraints that define the feasible re-

Correspondence concerning this article should be addressed to J. D. Perkins.

gion of operation. These constraints originate from product quality specifications, safety related aspects, operational requirements and environmental regulations, and can be posed as constraints on the maximum, time domain deviation of certain process variables.

Rijnsdorp (1967), Maarleveld and Rijnsdorp (1970), and Lee and Weekman (1976) were among the first to discuss the important implications of the second set of control objectives for the economic performance of a process. They investigated, through a number of industrial case studies, the operational difficulties arising from the fact that the operating point is in most cases defined by the intersection of several constraints on variables that belong to the second category of control objectives. Reduction of the variability of variables close to these constraints was identified as a key aspect in any attempt to increase process profitability. Thus, the variability of certain process variables can directly be related to the economic performance of a plant and seen as part of the objective function.

Based on the impact of disturbances on the economic performance of a plant, Perkins (1989), Narraway et al. (1991), Narraway and Perkins (1993), and Perkins and Walsh (1996) presented variations on a method that yields an economic performance index that allows the design engineer to unambiguously rank control structure alternatives. This is an optimization-based approach where the economic cost of disturbances, acting at specified frequencies, is evaluated as a function of the control structure employed. Integer variables are introduced in order to model the alternatives.

In this study an extension of this previous work is presented. Approximate bounds on the maximum time domain deviation of the main process variables are calculated under closed-loop conditions. In addition, the range of discrete frequencies considered in this previous work is replaced by the worst case combination of disturbance frequencies. Furthermore, the assumption of perfect control at all frequencies of interest is relaxed and realistic, decentralized PI controllers are included in the proposed formulation. A number of case studies are presented including an evaporator, a reactive distillation column, and a reactor separator process.

## Process Synthesis Problem and Concept of Back-Off

The mathematical formulation of the process synthesis problem for continuous plants can be stated as follows (Mohideen et al., 1996)

$$\begin{aligned} \min_{u(t),\,d,\,X} \quad & E\left[J(x(t), z(t), p(t), u(t), d, X)\right] \\ \text{s.t.} \quad & h_D(\dot{x}(t), x(t), z(t), p(t), u(t), d, X) = \mathbf{0} \\ & h_A(x(t), z(t), p(t), u(t), d, X) = \mathbf{0} \\ & g(x(t), z(t), p(t), u(t), d, X) \leq \mathbf{0} \\ & x(t) \in X, z(t) \in Z, p(t) \in P \\ & u(t) \in U, d \in D, t \in T, X \in \{0,1\}^{n_X} \end{aligned} \qquad \text{(P1)}$$

where $x(t)$ is the $n_x$ vector of differential variables, $z(t)$ is the $n_z$ vector of algebraic variables, $p(t)$ is the $n_p$ vector of uncertain parameters, $u(t)$ is the $n_u$ vector of control variables (variables that can change during operation), $d$ is the $n_d$ vector of design variables, and $X$ is the vector of integer variables associated with the decisions that define the topology of the process (including that of the controller). $h_D$ and $h_A$ are the $n_x$, $n_z$ vectors of differential and algebraic equations that describe the dynamic behavior of the system and $g$ is the $n_g$ vector of inequality constraints that define the region of feasible operation of the plant. $J$ is the objective function whose expected value $(E)$ is to be minimized and $T$ is the time period over which the optimization is carried out. Given a set of appropriate initial conditions, the above problem aims to choose the optimal process topology $(X)$, the optimal process design $(d)$, as well as an operating point $(u(t))$ that will minimize the expected value of the goal function $(E(J(.))$ and at the same time satisfy the feasibility constraints $(g(.))$ over the time horizon $t \in T$ $(=[0,\infty)$ in most cases). Therefore, it is an infinite dimensional, dynamic optimization problem. Attempts to solve even simplified versions of this problem have only recently appeared in the literature (Narraway and Perkins, 1994; Dimitriadis and Pistikopoulos, 1995; Mohideen et al., 1996; Perkins and Walsh, 1996; Figueroa et al., 1996; Bahri et al., 1996).

The uncertain parameters can be decomposed into two subsets depending on their time scales. The first set contains the uncertain parameters with time scales considerably longer than the time scale of the process (low frequency disturbances). The effect of these disturbances is, in most cases, to change the optimum operating point of the plant and thus require the corrective action of an on-line, steady-state optimization algorithm. The second set contains the uncertain parameters with time scales comparable to the time scale of the process (high frequency disturbances). These parameters do not change the optimum operating point, but their effect is to constantly move the actual operation point in a (closed) region that surrounds the optimum operating point. The uncertain parameters are replaced in the formulation of the process synthesis problem by their nominal values. Thus, the expectation term can be dropped, but, more importantly, the time horizon of interest is now restricted to the steady state. Thus, problem P1 is simplified to

$$\begin{aligned} \min_{u,\,d,\,Y} \quad & J(x, z, p, u, d, Y) \\ \text{s.t.} \quad & h_D(x, z, p, u, d, Y) = \mathbf{0} \\ & h_A(x, z, p, u, d, Y) = \mathbf{0} \\ & g(x, z, p, u, d, Y) \leq \mathbf{0} \\ & x \in X, z \in Z, u \in U, d \in D \\ & Y \in \{0,1\}^{n_Y}, \quad p = p_N \end{aligned} \qquad \text{(P2)}$$

where $Y$ is obtained from $X$ by eliminating all integer variables that correspond to structural decisions related to the control system design. The solution of the MINLP problem P2 gives the optimum design, as well as the optimum operating point. However, the performance of the actual process is described by problem P1. If we assume that the optimal steady-state operating point is defined by the intersection of active constraints (as shown in Figure 1 for the case of 2 degrees of freedom), then any disturbance is likely to produce plant operation in the infeasible region. Thus, in order to avoid dynamic infeasibility we need to modify problem P2 so that the plant satisfies the constraints under the effect of un-

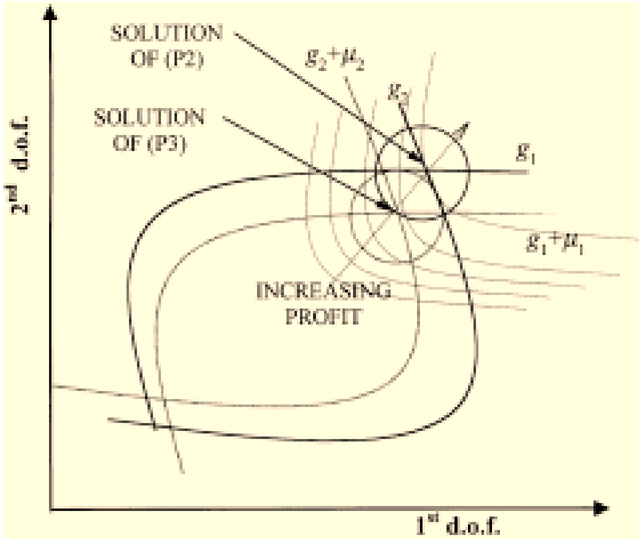


**Figure 1. Dynamic and steady-state process economics.**

certainty. To this end, we define the following quantities

$$\mu_l = \max_{\substack{t \in T \\ p(t) \in P}} \left( g_l(x, z, p, u, d, X) \right) - g_l(x_N, z_N, p_X, u_N, d_N, X), \quad \forall l, l = 1, 2, \ldots, n_g \quad (1)$$

that is, $\mu_l$ is the maximum violation of the $l$-th constraint over the time horizon of interest (the subscript $N$ denotes nominal value). Then, by using this information we can modify problem P2 to the form

$$\begin{aligned} &\min_{u, d, Y} J(x, z, p, u, d, Y) \\ \text{s.t.}\ & h_D(x, z, p, u, d, Y) = \mathbf{0} \\ & h_A(x, z, p, u, d, Y) = \mathbf{0} \\ & g(x, z, p, u, d, Y) + \boldsymbol{\mu} \leq \mathbf{0} \\ & x \in X, z \in Z, u \in U \\ & d \in D, \quad Y \in \{0, 1\}^{n_Y}, \quad p = p_N \end{aligned} \quad \text{(P3)}$$

This formulation ensures that its solution will give a new nominal operating point for which the plant operation will remain feasible for the whole set of uncertainty. This is illustrated in Figure 1. The solution of problem P2 defines the steady-state economics, while the solution of the problem P3 defines the dynamic economics of the process.

It should be noted that, since the feasible region of problem P3 is a subset of the feasible region of problem P2, the following holds true

$$\delta J = J_{(P3)} - J_{(P2)} \cong \sum_{l \in I_A} \lambda_l \mu_l \geq 0 \quad (2)$$

that is, the dynamic economics is bounded from below by the steady-state economics. Furthermore, using information obtained from the optimality conditions of problem P2, namely, the Lagrange multipliers $\lambda_l$, we can obtain an estimate of the economic giveaway necessary to mitigate the effects of disturbances. However, the actual value of $\delta J$ can be obtained by solving problem P3. Nevertheless, Eq. 2 clearly shows that the economic giveaway depends strongly on the size of constraint back-offs given by the vector $\boldsymbol{\mu}$. Therefore, the amount of back-off required to ensure feasible dynamic operation is a crucial factor and a method for its calculation has to be devised. The size of the back-off depends on the regulatory control system implemented (its structure and parameters), the disturbance characteristics (magnitude and frequency), and plant design (topology and design parameters). The first two factors are the more complicating ones. Since the size of the back-off depends on the structure and the parameters of the regulatory control system, the design of an "optimal" regulatory controller has to be carried out prior to the estimation of the amount of back-off. This requires decisions to be made about the control objectives and their realization, the type of controller to be used, and the specific technique for designing its parameters. This is far from a trivial task. The second factor is related to the characteristics of the disturbances. However, only limited information can be available about the disturbance characteristics prior to the real plant operation. Thus, in looking for a method for estimating the size of back-off one must have in mind that this method should give answers to an incompletely defined problem and that the subproblems involved are of high complexity.

## Linearization at the Optimum Steady State

In this section the linearization of the system dynamics is performed. To this end, we consider the problem that is obtained from problem P1 by assuming that the disturbances obtain their nominal values and that the design variables (including the binary variables) are fixed

$$\begin{aligned} &\min_{u} J(x, z, p, u) \\ \text{s.t.}\ & h_D(\dot{x}, x, z, p, u) = \mathbf{0} \\ & h_A(x, z, p, u) = \mathbf{0} \\ & g(x, z, p, u) \leq \mathbf{0} \\ & x_L \leq x \leq x_U,\ z_L \leq z \leq z_U \\ & u_L \leq u \leq u_U,\ p = p_N,\ \dot{x} = \mathbf{0} \end{aligned} \quad (3)$$

The solution of this problem defines the optimum steady-state operating point denoted by the subscript $N$ ($x_N$, $z_N$, $u_N$). The dynamics of the process close to this nominal point can be described with adequate accuracy by the linearization of the Eq. 3 at the nominal point

$$\begin{aligned} &\left(\frac{\partial h_D}{\partial \dot{x}}\right)\delta \dot{x} + \left(\frac{\partial h_D}{\partial x}\right)\delta x + \left(\frac{\partial h_D}{\partial z}\right)\delta z + \left(\frac{\partial h_D}{\partial u}\right)\delta u + \left(\frac{\partial h_D}{\partial p}\right)\delta p = \mathbf{0} \\ &\left(\frac{\partial h_A}{\partial x}\right)\delta x + \left(\frac{\partial h_A}{\partial z}\right)\delta z + \left(\frac{\partial h_A}{\partial u}\right)\delta u + \left(\frac{\partial h_A}{\partial p}\right)\delta p = \mathbf{0} \\ &g_N + \left(\frac{\partial g}{\partial x}\right)\delta x + \left(\frac{\partial g}{\partial z}\right)\delta z + \left(\frac{\partial g}{\partial u}\right)\delta u + \left(\frac{\partial g}{\partial p}\right)\delta p \leq \mathbf{0} \end{aligned} \quad (4)$$

where $\delta$ stands for deviation from the nominal point (such as $\delta x = x - x_N$ ). Assume that $h_D$, and $h_A$ constitute a differential-algebraic equations (DAE) system of index not exceeding 1 (Brenan et al., 1989), for which the matrix

$$\begin{bmatrix} \left(\frac{\partial h_D}{\partial \dot{x}}\right) & \left(\frac{\partial h_D}{\partial z}\right) \\ \mathbf{0} & \left(\frac{\partial h_A}{\partial z}\right) \end{bmatrix} \tag{5}$$

is nonsingular. Then, Eq. 4 can be written as

$$\begin{aligned} -I\delta\dot{x} + A\delta x + B\delta u + F\delta p &= \mathbf{0} \\ g_N + H\delta x + P\delta u + S\delta p &\le \mathbf{0} \end{aligned} \tag{6}$$

where

$$A \triangleq -\left(\frac{\partial h_D}{\partial \dot{x}}\right)^{-1}\left[\frac{\partial h_D}{\partial x} - \frac{\partial h_D}{\partial z}\left(\frac{\partial h_A}{\partial z}\right)^{-1}\left(\frac{\partial h_A}{\partial x}\right)\right] \tag{7}$$

$I$ is the identity matrix and $B$, $F$, $H$, $P$, and $S$ are defined analogously to $A$. Finally, we define the vector $\sigma$ as the vector of deviations of the inequality constraints from their nominal value

$$\sigma \triangleq g - g_N \tag{8}$$

Since for points close to the nominal point the following holds true

$$g \approx g_N + H\delta x + P\delta u + S\delta p \le \mathbf{0} \tag{9}$$

Equation 8 can be written as

$$-I\sigma + H\delta x + P\delta u + S\delta p = \mathbf{0} \tag{10}$$

Comparing Eq. 8 with Eq. 1, we observe that the maximum value of $\sigma_l$ is a linear, local approximation to the exact value of the maximum constraint deviation denoted by $\mu_l$. Thus, the following linear model can be used to estimate the necessary open-loop (without control) back-off

$$\begin{aligned} -I\delta\dot{x} + A\delta x + B\delta u + F\delta p &= \mathbf{0} \\ -I\sigma + H\delta x + P\delta u + S\delta p &= \mathbf{0} \end{aligned} \tag{11}$$

by assuming that

$$\mu_l \approx \rho_l \triangleq \max_{\substack{t\in T \\ p(t)\in P}} |\sigma_l(t)|, \quad \forall l,\ l = 1,2,\ldots,n_g \tag{12}$$

This is a dynamic optimization problem that can be avoided by transforming the problem into the frequency domain. To this end, a bounding property connecting the maximum deviation in the time domain with the maximum of the magnitude in the frequency domain is presented.

## Frequency Response Bounds to Step Disturbances

Heath et al. (1996) and Owen (1996) have demonstrated that an upper bound in the frequency domain can be developed for the vector $\rho$ (see Eq. 12). They have shown that for single input, single output (SISO) systems, the maximum of the magnitude curve over the frequency domain is an upper bound for the maximum of the step response of the system

$$\max_t \left| L^{-1}\left(\frac{\delta p}{s} g(s)\right)\right| \le f_s \max_\omega |g(j\omega)| \cdot |\delta p| \tag{13}$$

where $L^{-1}$ is the inverse Laplace transform, $f_s$ is a scaling factor that depends on the type of the system (considered as equal to one in the following for simplicity), and $g(s)$ a SISO transfer function. For the case of multi-input, multi-output (MIMO) systems, due to the principle of superposition, the following bound also holds

$$\max_t |\delta y_i(t)| \le \sum_j \max_\omega |g_{ij}(j\omega)| \cdot |\delta p_j| \tag{14}$$

where

$$\delta y_i(s) = \sum_j g_{ij}(s)\delta p_j(s), \quad \forall i \tag{15}$$

It should be noted that Eq. 14 is also valid for systems with time delay since the magnitude of the time delay is one for all frequencies.

Before closing this section, it should be noted that the use of the inequality given by Eq. 14 restricts the applicability of the proposed method to systems that exhibit stable open-loop dynamics. This is due to the fact that the step response of an integrating or unstable system is not bounded. Thus, the assumptions that need to be fulfilled for the application of the proposed methodology are the following: (a) the open-loop dynamics of the system is described by a DAE system of index not exceeding one; (b) the $A$ matrix defined in Eq. 7 has negative eigenvalues.

## Control Structure Selection Based on Perfect Control

In this section, the linear deviation model of the system given by Eq. 11 will be combined with a mathematical description of the perfect controller in order to develop a method for estimating the closed-loop constraint back-off. Equation 11 describes the dynamics of the system and the deviations of the inequality constraints from their nominal values, close to the steady-state optimal point, under the effect of uncertainty. However, this is an open-loop description since no controller is included. Thus, a method has to be devised that would invent the optimal, regulatory controller and then its state space description can be used together with Eq. 11 in order to estimate the necessary constraint back-off. In order to overcome the complicating nature of this problem, Narraway and Perkins (1993) proposed the use of the perfect control assumption.

Firstly, a set of potential controlled variables has to be defined. This set is a subset of the state vector and can be defined as follows

$$\delta y = C\,\delta x \tag{16}$$

Putting Eq. 16 together with Eq. 11 and decomposing into real and imaginary parts, we obtain

$$\begin{aligned} AX^R + \omega I_x X^I + BU^R &= -FP^R \\ -I\Sigma^R + HX^R + PU^R &= -SP^R \\ IY^R - CX^R &= \mathbf{0} \\ -\omega IX^R + AX^I + BU^I &= \mathbf{0} \\ -I\Sigma^I + HX^I + PU^I &= \mathbf{0} \\ IY^I - CX^I &= \mathbf{0} \end{aligned} \tag{17}$$

where $X$, $U$, $P$, $\Sigma$ and $Y$ are the Laplace transforms of the $x$, $u$, $p$, $\sigma$, and $y$ vectors, superscript $R$ $(I)$ denotes the real (imaginary) part of a complex number, and $\omega$ denotes the frequency. The perfect control assumption implies that when a potential controlled variable is selected at the regulatory control level, then the controller will keep this variable at its set point irrespective of any other factor. If we use the set of binary variables $Z$ to denote the decisions associated with the selection of controlled variables, then the following inequalities can be used to impose the perfect control

$$\left.\begin{aligned} -y_{i,H} Z_i \le Y_i^R \le y_{i,H} Z_i \\ -y_{i,H} Z_i \le Y_i^I \le y_{i,H} Z_i \end{aligned}\right\} \forall i = 1,2,\ldots,n_y \tag{18}$$

When $Z_i = 0$, then Eq. 18 takes the form (perfectly controlled candidates)

$$Y_i^R = Y_i^I = 0 \tag{19}$$

and when $Z_i = 1$ then (acceptable variation of the uncontrolled candidates)

$$\begin{aligned} -y_{i,H} \le Y_i^R \le y_{i,H} \\ -y_{i,H} \le Y_i^I \le y_{i,H} \end{aligned} \tag{20}$$

We can associate a binary vector $W$ with the potential manipulated variables used in the regulatory control

$$\left.\begin{aligned} -u_{j,H} W_j \le U_j^R \le u_{j,H} W_j \\ -u_{j,H} W_j \le U_j^I \le u_{j,H} W_j \end{aligned}\right\} \forall j = 1,2,\ldots,n_u \tag{21}$$

When $W_j = 0$ then Eq. 21 takes the form (unused candidates)

$$U_j^R = U_j^I = 0 \tag{22}$$

and when $W_j = 1$ then (acceptable variation of the candidates used for control)

$$\begin{aligned} -u_{j,H} \le U_j^R \le u_{j,H} \\ -u_{j,H} \le U_j^I \le u_{j,H} \end{aligned} \tag{23}$$

Finally, in order to assure that the regulatory control structure selected corresponds to a square controller we impose the following equality constraint over the binary variables

$$\sum_{i=1}^{n_y} Z_i + \sum_{j=1}^{n_u} W_j = n_y \tag{24}$$

Equations 17, 18, 21, and 24 constitute a mixed-integer formulation of the perfectly controlled closed-loop system. For any feasible realization of the binary variables, this formulation can be used in order to obtain the frequency response of the closed-loop system that corresponds to the control structure defined by the binary variables. We are interested in calculating the maximum of the magnitude of the variables $\Sigma_l(s)$ over a frequency range

$$\max_{\omega \epsilon \Omega} \sqrt{\Sigma_l^R(\omega)^2 + \Sigma_l^I(\omega)^2}, \quad \forall l = 1,2,\ldots,n_g \tag{25}$$

However, this nonlinear calculation would transform our formulation to a MINLP problem. In order to preserve the linearity of the formulation we use the following lower bounds on the magnitude

$$\left.\begin{aligned} \Sigma_l^R(\omega_p) \le \epsilon_l \\ -\Sigma_l^R(\omega_p) \le \epsilon_l \\ \Sigma_l^I(\omega_p) \le \epsilon_l \\ -\Sigma_l^I(\omega_p) \le \epsilon_l \\ \sqrt{\left(\Sigma_l^R(\omega_p)\right)^2 + \left(\Sigma_l^I(\omega_p)\right)^2} \ge \epsilon_l \end{aligned}\right\} \begin{aligned} \forall l = 1,2,\ldots,n_l \\ p = 1,2,\ldots,n_\omega \end{aligned} \tag{26}$$

Furthermore, in order for these lower bounds to approximate tightly the maximum over the whole frequency range a multiperiod (or multifrequency) formulation was used. It is interesting to note that as the number of frequencies included in the formulation tends to infinity, $\epsilon$ approaches the maximum over the frequency domain with negligible error. Thus, at least in principle, no accuracy is lost by this discretization of the frequency space. However, as the number of periods is increased, the size and the complexity of the underlying problem is also drastically increased.

Having a method to calculate the back-off vector that corresponds to each control structure, then, using Eqs. 6 and 16, we can calculate the economic penalty associated with this back-off vector by solving the following LP

$$\begin{aligned} \min_u\ & \boldsymbol{\alpha}^T \delta x + \boldsymbol{\beta}^T \delta u \\ & A\,\delta x + B\,\delta u = \mathbf{0} \\ & I\,\delta y - C\,\delta x = \mathbf{0} \\ & g_N + H\,\delta x + P\,\delta u \le -I\boldsymbol{\rho} \\ & u_L \le u \le u_U \end{aligned} \tag{27}$$

where $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$ are the gradients of the objective function with respect to the state and control variables, respectively. Finally, in order to select the best control structure, the structure that corresponds to the minimum economic penalty, we have to solve the following MILP problem

$$\min_u \boldsymbol{\alpha}^T \delta x + \boldsymbol{\beta}^T \delta u$$

$$A\,\delta x + B\,\delta u = \mathbf{0}$$

$$I \delta y - C \delta x = \mathbf{0}$$

$$g_N + H \delta x + P \delta u \leq - I \boldsymbol{\rho}$$

$$u_L \leq u \leq u_U$$

$$\sum_{i=1}^{n_y} Z_i + \sum_{j=1}^{n_u} W_j = n_y \tag{28}$$

$$\left.\begin{array}{r} AX^R + \omega_p IX^I + BU^R = -FP^R \\ -I\Sigma^R + HX^R + PU^R = -SP^R \\ IY^R - CX^R = \mathbf{0} \\ -\omega_p IX^R + AX^I + BU^I = \mathbf{0} \\ -I\Sigma^I + HX^I + PU^I = \mathbf{0} \\ IY^I - CX^I = \mathbf{0} \\ \left.\begin{array}{r} -y_{i,H} Z_i \leq Y_i^R \leq y_{i,H} Z_i \\ -y_{i,H} Z_i \leq Y_i^I \leq y_{i,H} Z_i \end{array}\right\} \forall i \\ \left.\begin{array}{r} -u_{j,H} W_j \leq U_j^R \leq u_{j,H} W_j \\ -u_{j,H} W_j \leq U_j^I \leq u_{j,H} W_j \end{array}\right\} \forall j \\ \left.\begin{array}{r} \Sigma_l^R \leq \epsilon_l \\ -\Sigma_l^R \leq \epsilon_l \\ \Sigma_l^I \leq \epsilon_l \\ -\Sigma_l^I \leq \epsilon_l \\ \epsilon_l \leq \rho_l \end{array}\right\} \forall l \end{array}\right\} \forall p$$

This formulation assumes that a model of the form given by Eq. 3 is available. However, in many cases such a detailed model may not be available. In these cases we can use an objective function of the form

$$\Delta J = \sum_i w_i^{\chi} \chi_i + \sum_j w_j^{\upsilon} \upsilon_j \tag{29}$$

where $w$ are weights that reflect the economic penalty that is related to the maximum deviations of the state ($\chi$) and control ($\upsilon$) variables. These maximum deviations can be calculated by applying the procedure used to calculate the maximum deviations of $\sigma$.

The formulation given by Eq. 28 is a mixed integer linear programming problem which determines the regulatory control structure that minimizes the economic penalty associated with the maximum time domain deviations of certain process variables. However, due to the fact that the estimated maxima over the frequency domain are only lower bounds on the real maxima, this formulation does not give (for each control structure defined by the binary variables) the actual objective function but only a lower bound on this objective function. This lower bound becomes increasingly tight as the number of discrete frequencies over which Eq. 28 is solved is increased. Nevertheless, the objective function obtained is a lower bound on the actual objective function and a modified MILP solution algorithm that takes this into consideration is presented in the following.

For any realization of the binary variables $Z_i$, Eq. 18 can be written in the following equivalent form

$$E_y Y = \mathbf{0} \tag{30}$$

In a similar way, for any realization of the binary variables $W_j$ we also have

$$E_u U = \mathbf{0} \tag{31}$$

Equations 30 and 31 together with the Laplace transform of Eqs. 11 and 16 constitute for each frequency the following set of $n_x + n_y + n_u + n_g$ equations in $n_x + n_u + n_y + n_g$ unknowns (Narraway et al., 1991)

$$\begin{bmatrix} X \\ U \\ Y \\ \Sigma \end{bmatrix} = \boldsymbol{\Phi}(j\omega) P \tag{32}$$

where

$$\tilde{\boldsymbol{\Phi}}(j\omega) = \begin{bmatrix} j\omega I_\chi & -A & -B & \mathbf{0} & \mathbf{0} \\ & -C & \mathbf{0} & I_y & \mathbf{0} \\ & -H & -P & \mathbf{0} & I_g \\ & \mathbf{0} & E_u & \mathbf{0} & \mathbf{0} \\ & \mathbf{0} & \mathbf{0} & E_y & \mathbf{0} \end{bmatrix}^{-1} \begin{bmatrix} F \\ \mathbf{0} \\ S \\ \mathbf{0} \\ \mathbf{0} \end{bmatrix} \tag{33}$$

In order to calculate the upper bounds on the maxima of the time domain deviations we define the following matrix

$$\tilde{\boldsymbol{\Phi}} = \left[ \tilde{\varphi}_{ij} \right] = \left\lfloor \max_{\omega \in \Omega} |\varphi_{ij}(\omega)| \right\rfloor \tag{34}$$

The frequency domain bounds can then be calculated as follows

$$\begin{bmatrix} \boldsymbol{\chi} \\ \boldsymbol{\upsilon} \\ \boldsymbol{\rho} \end{bmatrix} = \tilde{\boldsymbol{\Phi}} P \tag{35}$$

where $\boldsymbol{\chi}$, $\boldsymbol{\upsilon}$, and $\boldsymbol{\rho}$ are the vectors of actual upper bounds on the maximum time domain deviations of the state, input, and slack variables, respectively. Having calculated these bounds, the actual value of the objective function can be calculated using the LP formulation given by Eq. 27.

In order to solve the control structure selection problem, the MILP formulation given by Eq. 28 is solved to the first integer solution. Then, the actual value of the objective function is calculated based on Eqs. 27 and 35. This value is used as the entry cost at this integer solution and an integer cut is added to exclude the current integer solution from further consideration. In cases where no further integer solution can be found the algorithm has converged and the best entry cost corresponds to the global optimum. If no feasible integer solution can be found, then the problem is infeasible. The reader is referred to Williams (1985) for a comprehensive introduction to the terminology and solution of general MILP problems.

## Control Structure Selection Based on Realistic Controllers

In this section, a method for simultaneous selection of controlled and manipulated variables, variable pairing, and decentralized PI controller tuning is presented. To this end, consider the SISO transfer function relating input $j$ to output $i$ under PI control

$$U_j = g_{ji}^{PI}(-Y_i) \tag{36}$$

where

$$g_{ji}^{PI} = k_{ji}\left(1 + \frac{1}{\tau_{ji}s}\right) \tag{37}$$

$k_{ji}$ is the controller gain and $\tau_{ji}$ is the integral (or reset) time. We assume that these controller parameters can be calculated by considering each input-output pair and applying one of the well-known methods for SISO PI controller tuning (Marlin, 1995). However, these parameters can be totally inappropriate in a multivariable closed-loop system. In order to take the multivariable nature of the problem into consideration, Luyben (1990) suggested the use of a detuning factor $f$. Using this factor, the parameters of the decentralized PI controllers can be related to the values obtained by the SISO tuning procedures according to the following rules

$$k_{ji}^{\mathrm{MIMO}} = k_{ji}^{\mathrm{SISO}} f_{ji} \tag{38}$$

$$\tau_{ji}^{\mathrm{MIMO}} = \frac{\tau_{ji}^{\mathrm{SISO}}}{f_{ji}} \tag{39}$$

A method for calculating the detuning factors is also discussed by Luyben (1990). Upon substitution of Eqs. 38 and 39 into Eq. 37 we take

$$U_j = -k_{ji} f_{ji}\left(1 - j\frac{f_{ji}}{\tau_{ji}\omega}\right)Y_i \tag{40}$$

In general, it is desirable to have continuous detuning factors and calculate their optimal values as part of the algorithm. However, as can be observed from Eq. 40, using continuous detuning factors leads to the introduction of bilinear terms involving the detuning factors and the measured variables. In order to formulate a linear problem, which can be solved effectively to global optimality, the continuous detuning factors are replaced by a discrete set of values. This is done by introducing a discrete set of detuning factors $f_{jim}$ and a set of binary variables $\psi_{jim}$ that are used to select the particular discrete detuning factor according to: $\psi_{jim} = 1$ implies that $f_{jim}$ is the detuning factor used in $j$-$i$ channel, $\psi_{jim} = 0$ implies that $f_{jim}$ detuning factor is not used in $j$-$i$ channel.

Since only square, decentralized controllers are considered in this work, the following constraints on the binary variables must hold

$$\sum_i \sum_m \psi_{jim} \le 1, \quad \forall j \tag{41}$$

$$\sum_j \sum_m \psi_{jim} \le 1, \quad \forall i \tag{42}$$

Equation 41 imposes the constraint that, at most, one potential controlled variable is assigned to each potential manipulated variable, and Eq. 42 that, at most, one potential manipulated variable is assigned to each potential controlled variable. It should further be noted that $\sum_i \sum_m \psi_{jim} = 0$ means that the potential manipulated variable $u_j$ is not used in the control structure while, when $\sum_j \sum_m \psi_{jim} = 0$ the potential controlled variable, $y_i$ is not used in the control structure.

Using these integer variables and discrete detuning factors, Eq. 40 can be written in the following form

$$U_j = \sum_i \sum_m (-k_{ji}) f_{jim} \psi_{jim}\left(1 - j\frac{f_{jim}}{\tau_{ji}\omega}\right)Y_i \tag{43}$$

We further define the following discrete controller gains and transformed measurements

$$K_{jim} = -k_{ji} f_{jim} \tag{44}$$

$$Y_{jim}^R = Y_i^R + \frac{f_{jim}}{\tau_{ji}\omega} Y_i^I \tag{45}$$

$$Y_{jim}^I = Y_i^I - \frac{f_{jim}}{\tau_{ji}\omega} Y_i^R \tag{46}$$

Using Eqs. 44–46, Eq. 43 becomes

$$U_j^R = \sum_i \sum_m K_{jim} \psi_{jim} Y_{jim}^R, \quad \forall j \tag{47}$$

$$U_j^I = \sum_i \sum_m K_{jim} \psi_{jim} Y_{jim}^I, \quad \forall j \tag{48}$$

Equations 47 and 48 are nonlinear due to the multiplication of continuous and binary variables. Fortunately, this is one of the cases where efficient linearization techniques have been proposed. First, the following variables are introduced

$$\Gamma_{jim}^R = K_{jim} \psi_{jim} Y_{jim}^R \tag{49}$$

$$\Gamma_{jim}^I = K_{jim} \psi_{jim} Y_{jim}^I \tag{50}$$

and Eqs. 47 and 48 can be written in the following linear form

$$U_j^R = \sum_i \sum_m \Gamma_{jim}^R \tag{51}$$

$$U_j^I = \sum_i \sum_m \Gamma_{jim}^I \tag{52}$$

Finally, in order to enforce Eqs. 49 and 50 we assume that

$$-y_{i,H}^R \le Y_i^R \le y_{i,H}^R \tag{53}$$

then the following linear under- and over-estimators can be used (Glover, 1975)

$$\begin{aligned} -\Gamma_{jim}^R &\le \tilde{K}_{jim} Y_{ji,H}^R \psi_{jim} \\ \Gamma_{jim}^R &\le \tilde{K}_{jim} Y_{ji,H}^R \psi_{jim} \\ -\Gamma_{jim}^R &\le -K_{jim} Y_{jim}^R + \tilde{K}_{jim} Y_{ji,H}^R (1-\psi_{jim}) \\ \Gamma_{jim}^R &\le K_{jim} Y_{jim}^R + \tilde{K}_{jim} Y_{ji,H}^R (1-\psi_{jim}) \end{aligned} \tag{54}$$

where $\tilde{K}_{jim}$ denotes the absolute value of $K_{jim}$ and $Y_{ji,H}^R$ are upper bounds defined as follows

$$Y_{ji,H}^R = \left(1 + \frac{\max(f_{ji})}{\tau_{ij}\omega}\right) y_{i,H}^R \tag{55}$$

It should be noted that, when $\psi_{jim} = 0$, then Eq. 54 simplifies to

$$\Gamma_{jim}^R = 0 \tag{56}$$

while when $\psi_{jim} = 1$

$$\Gamma_{jim}^R = K_{jim} Y_{jim}^R \tag{57}$$

It is particularly important to incorporate the steady state ($\omega = 0$) in the formulation due to its significance. By using the property of perfect steady-state control that characterizes controllers with integral action, we can neglect the structure of the controller at zero frequency and use the plant model together with the perfect control constraints applied at that frequency, that is

$$\begin{aligned} &AX_0^R + BU_0^R = -FP^R \\ &-I\Sigma^R + HX_0^R + PU_0^R = -SP^R \\ &IY_0^R - CX_0^R = \mathbf{0} \\ &-u_{j,H}\left(\sum_i \sum_m \psi_{jim}\right) \le U_{0,j}^R \le u_{j,H}\left(\sum_i \sum_m \psi_{jim}\right), \quad \forall j \\ &-y_{j,H}\left(\sum_i \sum_m \psi_{jim}\right) \le Y_{0,i}^R \le y_{i,H}\left(1 - \sum_j \sum_m \psi_{jim}\right), \quad \forall i \end{aligned} \tag{58}$$

where the subscript 0 has been used in order to explicitly denote that these equations apply only at steady state. It should be noted that the imaginary parts of the variables have been eliminated from these steady-state constraints since, as can be seen by examining Eq. 17, they are identically zero at zero frequency. In summary, the following MILP formulation for the solution of the control structure selection problem with realistic, decentralized PI controllers is proposed

$$\begin{aligned} &\min_{u,\psi_{jim}} \ \boldsymbol{\alpha}^T \delta x + \boldsymbol{\beta}^T \delta u \\ &A\,\delta x + B\,\delta u = \mathbf{0} \\ &I\,\delta y - C\,\delta x = \mathbf{0} \\ &g_N + H\,\delta x + P\,\delta u \le -I\boldsymbol{\rho} \\ &u_L \le u \le u_U \\ &\sum_i \sum_m \psi_{jim} \le 1, \quad \forall j \\ &\sum_j \sum_m \psi_{jim} \le 1, \quad \forall i \\ &AX_0^R + BU_0^R = -FP^R \\ &-I\Sigma^R + HX_0^R + PU_0^R = -SP^R \\ &IY_0^R - CX_0^R = \mathbf{0} \\ &-u_{j,H}\left(\sum_i \sum_m \psi_{jim}\right) \le U_{0,j}^R \le u_{j,H}\left(\sum_i \sum_m \psi_{jim}\right), \quad \forall j \\ &-y_{i,H}\left(1-\sum_i \sum_m \psi_{jim}\right) \le Y_{0,i}^R \le y_{i,H}\left(1 - \sum_j \sum_m \psi_{jim}\right), \quad \forall i \\ &\left.\begin{aligned} AX^R + \omega_p IX^I + BU^R &= -FP^R \\ -I\Sigma^R + HX^R + PU^R &= -SP^R \\ IY^R - CX^R &= \mathbf{0} \\ -\omega_p IX^R + AX^I + BU^I &= \mathbf{0} \\ -I\Sigma^I + HX^I + PU^I &= \mathbf{0} \\ IY^I - CX^I &= \mathbf{0} \end{aligned}\right\} \forall p \\ &\left.\begin{aligned} U_j^R &= \sum_i \sum_m \Gamma_{jim}^R \\ U_j^I &= \sum_i \sum_m \Gamma_{jim}^I \end{aligned}\right\} \forall j, p \\ &\left.\begin{aligned} \Sigma_l^R &\le \epsilon_l \\ -\Sigma_l^R &\le \epsilon_l \\ \Sigma_l^I &\le \epsilon_l \\ -\Sigma_l^I &\le \epsilon_l \\ \epsilon_l &\le \rho_l \end{aligned}\right\} \forall l, \quad \forall p \\ &\left.\begin{aligned} -\Gamma_{jim}^R &\le \tilde{K}_{jim} Y_{ji,H}^R \psi_{jim} \\ \Gamma_{jim}^R &\le \tilde{K}_{jim} Y_{ji,H}^R \psi_{jim} \\ -\Gamma_{jim}^R &\le -K_{jim} Y_{jim}^R + \tilde{K}_{jim} Y_{ji,H}^R (1-\psi_{jim}) \\ \Gamma_{jim}^R &\le K_{jim} Y_{jim}^R + \tilde{K}_{jim} Y_{ji,H}^R (1-\psi_{jim}) \\ -\Gamma_{jim}^I &\le \tilde{K}_{jim} Y_{ji,H}^I \psi_{jim} \\ \Gamma_{jim}^I &\le \tilde{K}_{jim} Y_{ji,H}^I \psi_{jim} \\ -\Gamma_{jim}^I &\le -K_{jim} Y_{jim}^I + \tilde{K}_{jim} Y_{ji,H}^I (1-\psi_{jim}) \\ \Gamma_{jim}^I &\le K_{jim} Y_{jim}^I + \tilde{K}_{jim} Y_{ji,H}^I (1-\psi_{jim}) \\ Y_{jim}^R &= Y_i^R + \frac{f_{jim}}{\tau_{ji}\omega_p} Y_i^I \\ Y_{jim}^I &= Y_i^I - \frac{f_{jim}}{\tau_{ji}\omega_p} Y_i^R \end{aligned}\right\} \forall i, j, m, p \end{aligned} \tag{59}$$

The algorithm presented for the case of perfect control is also applied in the case of decentralized PI control since the calculated cost is a lower bound to the actual cost. In order to calculate the actual cost the worst case back-off is calculated first. Then the LP problem given by Eq. 27 is solved and its solution is used as the entry cost that corresponds to the current integer solution. However, Eqs. 30−35 were derived for the case of perfect control and, thus, they do not apply in the case of decentralized PI controllers. In what follows the calculation of the worst case back-off for the case of decentralized controllers is presented.

The system dynamics is described by Eqs. 11 and 16

$$\begin{aligned} -j\omega IX + AX + BU + FP &= \mathbf{0} \\ -I\Sigma + HX + PU + SP &= \mathbf{0} \\ IY - CX &= \mathbf{0} \end{aligned} \tag{60}$$

We then define the following variables as the integrals of the potential controlled variables

$$\dot{q} = y \tag{61}$$

or

$$j\omega Q - Y = \mathbf{0} \tag{62}$$

where $Q$ is the Laplace transform of $q$. Furthermore, define the $n_u$ by $n_y$ matrix $\Xi$ whose elements $\xi_{ji}$ are given by

$$\xi_{ji} = \sum_m f_{jim}\psi_{jim} \tag{63}$$

that is, each element of the matrix $\Xi$ denotes whether or not the pairing *j-i* is part of the chosen structure and, at the same time, the value of the corresponding detuning factor. Then, the description of the PI controller that corresponds to the current integer solution is given by

$$U - E_K Y - E_I Q = \mathbf{0} \tag{64}$$

where

$$\begin{aligned} E_K &= K \otimes \Xi \\ E_I &= K \otimes T \otimes \Xi \\ K &= \left[k_{ji}\right], \quad T = \left[\tau_{ji}^{-1}\right] \end{aligned} \tag{65}$$

and $\otimes$ denotes element by element multiplication (Schur product). Equations 60, 62, and 64 constitute, at each frequency, the following system of $n_x + n_g + 2n_y + n_u$ linear equations in $n_x + n_g + 2n_y + n_u$ unknowns

$$\begin{bmatrix} -j\omega I - A & -B & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ -H & -P & \mathbf{0} & I_g & \mathbf{0} \\ -C & \mathbf{0} & I_y & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & I_y & \mathbf{0} & -j_w I_y \\ \mathbf{0} & I_u & -E_K & \mathbf{0} & -E_I \end{bmatrix} \begin{bmatrix} X \\ U \\ Y \\ \Sigma \\ Q \end{bmatrix} = \begin{bmatrix} F \\ \mathbf{0} \\ S \\ \mathbf{0} \\ \mathbf{0} \end{bmatrix} P \tag{66}$$

This set of equations is of the same form as the one presented for the case of perfect control given by Eq. 32. Thus, the maximum constraint back-off can be calculated as indicated by Eq. 35.

## Solution Algorithm

In this section, a decomposition approach that can accelerate the solution of problem given by Eq. 59 is presented. The necessity of this decomposition approach is due to the fact that the number of alternatives that has to be taken into consideration, even for small problems, is extremely large. This number can be calculated using the following

$$N_S = \sum_{k=1}^{N} \binom{n_u}{k}\binom{n_y}{k} k!\, n_t^k = \sum_{k=1}^{N} \frac{n_u!}{k!(n_u-k)!}\frac{n_y!}{k!(n_y-k)!} k!\, n_t^k \tag{67}$$

where $N = \min\{n_u, n_y\}$ and $N_S$ is the number of alternative solutions.

In order to apply the proposed algorithm more effectively, a decomposition is used that is based on the idea of separating the problem of selecting sets of controlled and manipulated variables from the pairing and tuning problem. This is achieved by first solving the following steady state, perfect control problem that is derived from Eq. 28 by eliminating the imaginary parts of variables

$$\begin{gathered} \min_{Z,W,u} \boldsymbol{\alpha}^T \delta x + \boldsymbol{\beta}^T \delta u \\ A\,\delta x + B\,\delta u = \mathbf{0} \\ I\,\delta y - C\,\delta x = \mathbf{0} \\ Ig_N + H\,\delta x + P\,\delta u \le -I_g\,\boldsymbol{\rho} \\ -u_L \le u \le u_U \\ \sum_{i=1}^{n_y} Z_i + \sum_{j=1}^{n_u} W_j = n_y \\ AX^R + BU^R = -FP^R \\ -I\Sigma^R + HX^R + PU^R = -SP^R \\ IY^R - CX^R = \mathbf{0} \\ -y_{i,H}Z_i \le Y_i^R \le y_{i,H}Z_i, \quad \forall i \\ -u_{j,H}W_j \le U_j^R \le u_{j,H}W_j, \quad \forall j \\ \left.\begin{aligned} \Sigma_l^R &\le \epsilon_l \\ -\Sigma_l^R &\le \epsilon_l \\ \epsilon_l &\le \rho_l \end{aligned}\right\} \forall l \end{gathered} \tag{68}$$

Then, for each structure chosen by the solution of the problem given by Eq. 68, the problem given by Eq. 59 is solved by imposing the constraints

$$\sum_i \sum_m \psi_{jim} = 1, \quad \forall j \in J_A = \{ j: Z_j = 1 \}$$

$$\sum_j \sum_m \psi_{jim} = 1, \quad \forall i \in I_A = \{ i: W_i = 0 \} \tag{69}$$

In order to reduce the number of feasible alternative solutions at this variable pairing and tuning step the following constraints are also used

$$\lambda_{ji} \left( \sum_m \psi_{jim} \right) \geq 0 \tag{70}$$

where $\lambda_{ji}$ is the $j$-$i$ element of the relative gain array defined as

$$\Lambda = [\lambda_{ji}] = G(0) \otimes [G^T(0)]^{-1} \tag{71}$$

and $G(0) = -CA^{-1}B$ is the steady-state gain matrix. Equation 70 imposes the well-known necessary condition for integral controllability with integrity (ICI) (Campo and Morari, 1994). Furthermore, systems that are not integral stabilizable (IS), that is, structures that do not satisfy the (necessary and sufficient) condition for IS (Campo and Morari, 1994)

$$\det[G(0)] \neq 0 \tag{72}$$

never enter the variable pairing and tuning step, and are excluded from further consideration by using integer cuts.

This decomposition has proven to be efficient in practice due to the fact that Eq. 68 can be solved easily to first integer solution even for large-scale problems, while the conditions given by Eqs. 71 and 72 eliminate a substantial number of alternatives that do not satisfy the IS or ICI conditions.

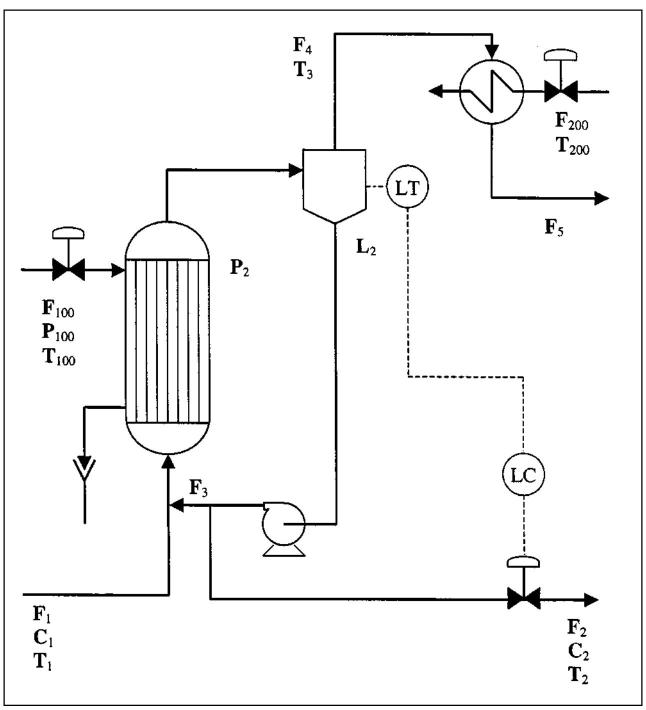


**Figure 2. Evaporator system.**

## Case Studies

### *Case study 1: Evaporation process model*

The evaporation process examined in this section is shown in Figure 2. This is a process which removes a volatile liquid from a nonvolatile solute, thus concentrating the solution. It consists of a heat exchange vessel with a recirculating pump. The overhead vapor is condensed by the use of a process heat exchanger. The major variables of interest are summarized in Table 1. The details of the mathematical model can be found in Newell and Lee (1989). The final form of the dynamic model is given by

$$\rho A \frac{dL_2}{dt} = F_1 - F_4 - F_2 \tag{73}$$

$$M \frac{dC_2}{dt} = F_1 C_1 - F_2 C_2 \tag{74}$$

$$C \frac{dP_2}{dt} = F_4 - F_5 \tag{75}$$

where

$$F_4 = \{ 0.16(F_1 + F_3) \times (-0.3126 C_2 - 0.5616 P_2 + 0.1538 P_{100} + 41.57) - F_1 C_p (0.3126 C_2 + 0.5616 P_2 + 48.43 - T_1) \} / \lambda_{s1} \tag{76}$$

$$F_5 = \frac{2UA_2 (0.507 P_2 + 55 - T_{200}) C_p F_{200}}{\lambda_{s2} (UA_2 + 2 C_p F_{200})} \tag{77}$$

In the above equations $\rho A$ is the product of liquid density and the cross-sectional area of the evaporator (20 kg/m), $M$ is the liquid holdup in the evaporator (20 kg), $C$ is a constant (4 kg/kPa), $UA_2$ is the product of the heat-transfer coefficient and the heat-transfer area in the condenser (6.84 kW/K), $C_p$ is the heat capacity of the cooling water (0.07 kW/kg·min), $\lambda_{s1}$ is the latent heat of steam at saturated conditions (36.6 kW/min·kg) and $\lambda_{s2}$ is the latent heat of evaporation of water (38.5 kW/kg·min).

The operating cost of the evaporator consists of the cost of electricity, the cost of steam, and the cost of cooling water (Wang and Cameron, 1994)

**Table 1. Major Variables of the Evaporation Process Model**

| | |
|---|---|
| $F_1$=feed flow rate (kg/min) | $T_3$=vapor temperature |
| $F_2$=product flow rate | $T_{100}$=steam temperature |
| $F_3$=circulation flow rate | $T_{200}$=cooling water inlet temperature |
| $F_4$=vapor flow rate | $T_{201}$=cooling water outlet temperature |
| $F_5$=condensate flow rate | $C_1$=feed composition (%) |
| $F_{100}$=steam flow rate | $C_2$=product composition |
| $F_{200}$=cooling water flow rate | $P_2$=operating pressure (kPa) |
| $T_1$=feed temperature (°C) | $P_{100}$=steam pressure |
| $T_2$=product temperature | $L_2$=separator level (m) |

**Table 2. Results for Case 1 (Evaporator Model - Perfect Control)**

| | $\epsilon_1$ | $\epsilon_2$ | $\epsilon_3$ | $\epsilon_4$ | $\epsilon_5$ | $\delta x_1$ | $\delta x_2$ | $\delta u_1$ | $\delta u_2$ | $\Delta J \times 10^{-3}$ |
|---|---|---|---|---|---|---|---|---|---|---|
| Open Loop | 7.34 | 4.61 | 4.61 | 0.00 | 0.00 | | | | | $+\infty$ |
| (u1, u2)−(y1, y2) | 0.00 | 0.00 | 0.00 | 11.90 | 91.06 | 0.00 | −2.90 | −11.89 | 33.04 | 0.0011 |
| u1−y1 | 0.00 | 8.01 | 8.01 | 44.69 | 0.00 | | | | | $+\infty$ |
| u1−y2 | 14.57 | 0.00 | 0.00 | 52.18 | 0.00 | | | | | $+\infty$ |
| u2−y1 | | | | | | | | | | $+\infty$ |
| u2−y2 | 3.19 | 0.00 | 0.00 | 0.00 | 88.98 | 3.00 | −2.91 | 0.00 | 51.79 | 0.0966 |

$$J = 1.009(F_2 + F_3) + \frac{96(F_1 + F_3)(T_{100} - T_2)}{\lambda_{s1}} + 0.6F_{200} \quad \text{in (\$/h)} \tag{78}$$

where

$$T_{100} = 0.1538P_{100} + 90 \tag{79}$$

$$T_2 = 0.5616P_2 + 0.3126C_2 + 48.43 \tag{80}$$

The inequality constraints that define the region of feasible operation are the following

$$g_1 = -C_2 + 35 \le 0 \tag{81}$$

$$g_2 = 40 - P_2 \le 0 \tag{82}$$

$$g_3 = P_2 - 80 \le 0 \tag{83}$$

$$g_4 = P_{100} - 400 \le 0 \tag{84}$$

$$g_5 = F_{200} - 400 \le 0 \tag{85}$$

The process is open-loop unstable due to the integrating behavior of the Eq. 73. Thus, in order to make the system open-loop stable we introduce the algebraic equation

$$F_2 = F_1 - F_4 \tag{86}$$

corresponding to perfect control of the level in the overhead drum ($L_2$) that eliminates the first differential equation. We further define the following vectors

$$x = y = \begin{bmatrix} C_1 \\ P_2 \end{bmatrix}, \quad u = \begin{bmatrix} P_{100} \\ F_{200} \end{bmatrix}, \quad p = \begin{bmatrix} F_1 \\ C_1 \\ T_1 \\ T_{200} \end{bmatrix} \tag{87}$$

In order to find the optimum point of steady-state operation we consider the following input conditions

$$F_1 = 10 \text{ kg/min}, \quad C_1 = 5\%, \quad T_1 = 40°C, \quad T_{200} = 25°C \tag{88}$$

The objective function is optimized, subject to the equality as well as the inequality, constraints. The optimum operating point is the following

$$x_N = \begin{bmatrix} x_{1,N} \\ x_{2,N} \end{bmatrix} = \begin{bmatrix} 35.0000 \\ 56.2079 \end{bmatrix} \tag{89}$$

$$u_N = \begin{bmatrix} u_{1,N} \\ u_{2,N} \end{bmatrix} = \begin{bmatrix} 400.000 \\ 229.925 \end{bmatrix} \tag{90}$$

and the optimum objective function is 5891.6 (\$/h). The constraints $g_1$ and $g_4$ are active at the optimum operating point and the corresponding Lagrange multipliers are $\lambda_1 = 0.032191$ and $\lambda_4 = 0.000092$. The linearized system is obtained directly from the calculated Jacobian of the constraints at the optimum operating point.

The perfect control formulation is applied first. In the case of the evaporation process model the number of alternative regulatory control structures is six: the open-loop structure, one $2 \times 2$ control structure, plus four $1 \times 1$ control structures. The calculations were carried out for three sets of values for the uncertain parameters

$$\delta p_1 = \begin{bmatrix} 0.1 \text{ kg} \\ 0.5\% \\ 4.0°C \\ 2.5°C \end{bmatrix}, \quad \delta p_2 = \begin{bmatrix} 0.05 \text{ kg} \\ 0.25\% \\ 2.0°C \\ 1.25°C \end{bmatrix}, \quad \delta p_3 = \begin{bmatrix} 0.01 \text{ kg} \\ 0.05\% \\ 0.4°C \\ 0.25°C \end{bmatrix} \tag{91}$$

The results are summarized in Table 2 (for $\delta p_1$), Table 3 (for

**Table 3. Results for Case 2 (Evaporator Model - Perfect Control)**

| | $\epsilon_1$ | $\epsilon_2$ | $\epsilon_3$ | $\epsilon_4$ | $\epsilon_5$ | $\delta x_1$ | $\delta x_2$ | $\delta u_1$ | $\delta u_2$ | $\Delta J \times 10^{-3}$ |
|---|---|---|---|---|---|---|---|---|---|---|
| Open Loop | 3.67 | 2.30 | 2.30 | 0.00 | 0.00 | | | | | $+\infty$ |
| (u1, u2)−(y1, y2) | 0.00 | 0.00 | 0.00 | 5.95 | 45.53 | 0.00 | −1.45 | −5.95 | 16.52 | 0.0005 |
| u1−y1 | 0.00 | 4.00 | 4.00 | 22.34 | 0.00 | 0.00 | −5.5 | −22.3 | 62.0 | 0.0021 |
| u1−y2 | 7.29 | 0.00 | 0.00 | 26.09 | 0.00 | | | | | $+\infty$ |
| u2−y1 | | | | | | | | | | $+\infty$ |
| u2−y2 | 1.51 | 0.00 | 0.00 | 0.00 | 44.93 | 1.50 | −1.45 | 0.00 | 28.89 | 0.0483 |

Table 4. Results for Case 3 (Evaporator Model - Perfect Control)

| | $\epsilon_1$ | $\epsilon_2$ | $\epsilon_3$ | $\epsilon_4$ | $\epsilon_5$ | $\delta x_1$ | $\delta x_2$ | $\delta u_1$ | $\delta u_2$ | $\Delta J \times 10^{-3}$ |
|---|---|---|---|---|---|---|---|---|---|---|
| Open Loop | 0.73 | 0.46 | 0.46 | 0.00 | 0.00 | 0.73 | −0.71 | 0.00 | 12.67 | 0.0236 |
| (u1, u2)−(y1, y2) | 0.00 | 0.00 | 0.00 | 1.19 | 9.11 | 0.00 | −0.29 | −1.18 | 3.30 | 0.0001 |
| u1−y1 | 0.00 | 0.80 | 0.80 | 4.46 | 0.00 | 0.00 | −1.09 | −4.46 | 12.41 | 0.0004 |
| u1−y2 | 1.45 | 0.00 | 0.00 | −5.21 | 0.00 | 1.45 | −2.68 | −5.21 | 39.64 | 0.0474 |
| u2−y1 | | | | | | | | | | $+\infty$ |
| u2−y2 | 0.30 | 0.00 | 0.00 | 0.00 | 8.89 | 0.30 | −0.29 | 0.00 | 5.17 | 0.0097 |

$\delta p_2$) and Table 4 (for $\delta p_3$). From these tables, we can conclude that:

- Decreasing the magnitude of the uncertainties generates more feasible structures, but the relative ranking of these structures is consistent.
- The calculated economic penalties can be predicted exactly by the simplified calculation given by Eq. 2.
- For the model evaporation process, the full control structure is the best structure followed by the $1\times1$ structure that controls perfectly the composition ($y_1$).

Finally, in Table 5 the calculated economic penalties for the formulations given by Eq. 28 (MILP formulation with approximate back-off) and Eqs. 27 and 35 (LP formulation with exact back-off) are compared. From this table, we can conclude that, for the example under consideration, the proposed algorithm will have a satisfactory performance. This is due to the fact that the optimum control structure has an economic penalty that is better than the approximate economic penalties of almost all other structures. Only one structure ($u_1$-$y_1$ structure) has a smaller approximate economic penalty.

The realistic controller-based MILP formulation was solved next only for case 2. The open-loop response was fitted to simple, first-order transfer functions, and the SISO PI controller parameters were calculated using the IMC tuning rules with an open-loop to closed-loop time constant ratio of three (Morari and Zafiriou, 1989). Five discrete detuning factors equally spaced between 0.1 and 1 were used, as well as two discrete frequencies $\omega_1 = 10^{-8}$ and $\omega_2 = 10^{-1}$. The optimum structure is given by the following $\Xi$ matrix

$$\Xi = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \tag{92}$$

that is, the best structure corresponds to the pairings $C_2$-$P_{100}$ and $P_2$-$F_{200}$ and both detuning factors equal to one. The back-off is given by the following vector

$$\boldsymbol{\rho} = \begin{bmatrix} 0.252 \\ 0.660 \\ 0.660 \\ 7.769 \\ 42.534 \end{bmatrix} \tag{93}$$

and the economic penalty is 8.8 (\$/h). This economic penalty is considerably greater than the economic penalty of the perfectly controlled system, although the control structure selected in both cases is the same. Using the nonlinear model of the evaporator process and the best control structure, the response of the closed-loop system to step disturbances of magnitude $\delta p_2$ is calculated. From these closed-loop simulations and the definition of the model constraints, we can calculate the exact value of the maximum deviation of the constraints from their nominal values (see the definition given by Eq. 1)

$$\boldsymbol{\mu} = \begin{bmatrix} 0.199 \\ 0.675 \\ 0.660 \\ 7.835 \\ 45.109 \end{bmatrix} \tag{94}$$

Comparing $\boldsymbol{\mu}$ given by Eq. 94 with $\boldsymbol{\rho}$ given by Eq. 93, we can see that a key assumption of this work (see Eq. 12) is clearly satisfied. The worst case combination of the maximum time domain deviations of the nonlinear, closed-loop model ($\boldsymbol{\mu}$) is well predicted by the worst case combination of the maximum magnitudes over the frequency domain ($\boldsymbol{\rho}$).

### *Case study 2: Reactive distillation for ethylene glycol synthesis.*

In this case study the double feed, reactive distillation column for ethylene glycol (EG) production presented by Ciric and Gu (1994) is considered. EG is produced from ethylene oxide (EO) and water (W)

$$\mathrm{EO} + \mathrm{W} \rightarrow \mathrm{EG}$$

EG reacts further with EO to produce the unwanted byproduct diethylene glycol (DEG)

$$\mathrm{EO} + \mathrm{EG} \rightarrow \mathrm{DEG}$$

Ciric and Gu (1994) present an optimal flowsheet for a double feed, reactive distillation column that consists of ten trays shown in Figure 3. The lower part of the distillation column (trays 1 to 4) is a simple separation zone, while the upper part (trays 5 to 10) is a reaction zone. Pure water is fed on tray 10, while pure ethylene oxide is fed on tray 5. A production rate specification of 25 kmol/h of EG is assumed. The modeling equations are presented in the following:

Table 5. Results for Case 3 (Evaporator Model-Perfect Control)

| | $\Delta J_{\mathrm{MILP}} \times 10^{-3}$ | $\Delta J_{\mathrm{LP}} \times 10^{-3}$ |
|---|---|---|
| Open Loop | 0.005614 | 0.023638 |
| (u1, u2)−(y1, y2) | 0.000057 | 0.000109 |
| u1−y1 | 0.000100 | 0.000412 |
| u1−y2 | 0.024719 | 0.047399 |
| u2−y1 | | |
| u2−y2 | 0.005040 | 0.009664 |

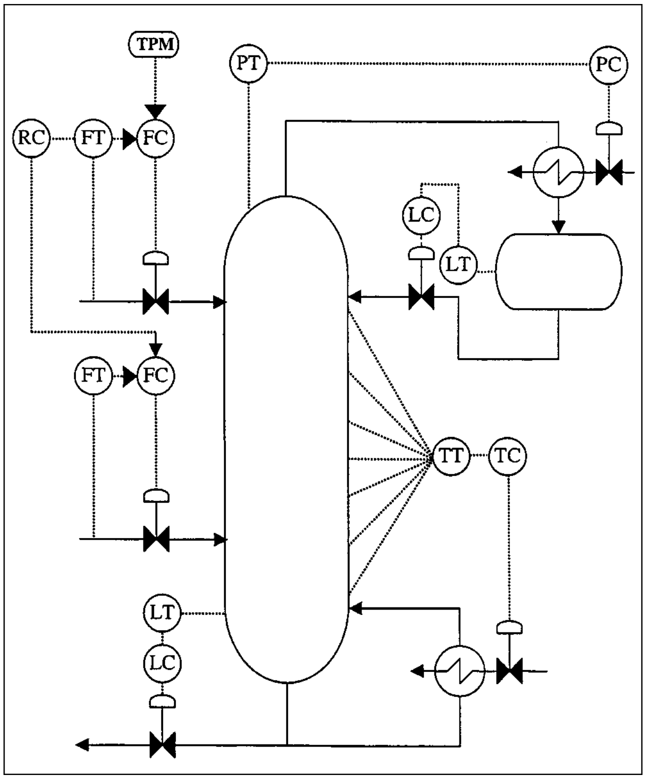


**Figure 3. Reactive distillation process.**

*Separation Section* ($j = 1, 2, 3, 4,\ i = 1, \ldots, N_C - 1$)

$$\frac{d}{dt}(M_j) = L_{j+1} - L_j - V_j + V_{j-1} \quad (95)$$

$$\frac{d}{dt}(M_j x_{ij}) = L_{j+1} x_{ij+1} - L_j x_{ij} - V_j y_{ij} + V_{j-1} y_{ij-1} \quad (96)$$

*Reaction Section* ($j = 6,7,8,9,\ i = 1,\ldots, N_C - 1$)

$$\frac{d}{dt}(M_j) = L_{j+1} - L_j - V_j + V_{j-1} - M_j \sum_{k=1}^{N_R} R_{jk} \quad (97)$$

$$\frac{d}{dt}(M_j x_{ij}) = L_{j+1} x_{ij+1} - L_j x_{ij} - V_j y_{ij} + V_{j-1} y_{ij-1} + M_j \sum_{k=1}^{N_R} n_{ik} R_{jk} \quad (98)$$

*Feed Trays* ($j = 5,10,\ i = 1, \ldots, N_C - 1$)

$$\frac{d}{dt}(M_j) = L_{j+1} - L_j - V_j + V_{j-1} + F_j - M_j \sum_{k=1}^{N_R} R_{jk} \quad (99)$$

$$\frac{d}{dt}(M_j x_{ij}) = L_{j+1} x_{ij+1} - L_j x_{ij} - V_j y_{ij} + V_{j-1} y_{ij-1} + F_j z_{ij} + M_j \sum_{k=1}^{N_R} n_{ik} R_{jk} \quad (100)$$

*Column Base* ($j = 0,\ i = 1, \ldots, N_C - 1$)

$$\frac{d}{dt}(M_j) = L_{j+1} - L_j - V_j \quad (101)$$

$$\frac{d}{dt}(M_j x_{ij}) = L_{j+1} x_{ij+1} - L_j x_{ij} - V_j y_{ij} \quad (102)$$

*Column Condenser and Reflux Drum* ($j = N_T + 1,\ i = 1, \ldots, N_C - 1$)

$$\frac{d}{dt}(M_j) = V_{j-1} - L_j \quad (103)$$

$$\frac{d}{dt}(M_j x_{ij}) = V_{j-1} y_{ij-1} - L_j x_{ij} \quad (104)$$

*Algebraic Equations*

$$L_j = c_o \rho_{Lj} l_W (h_{OW,j})^{3/2}, \quad j = 1, 2, \ldots, 10 \quad (105)$$

$$M_j = (h_W + h_{OW,j}) \left(\frac{\pi D_C^2}{4}\right) \left(\frac{\rho_{Lj}}{MW_{Lj}}\right), \quad j = 1, 2, \ldots, 10 \quad (106)$$

$$(V_j - V_{j-1}) \Delta H_{VAP} - M_j \sum_{k=1}^{N_R} R_{jk} \Delta H_k^R = 0, \quad j = 1, 2, \ldots, 10 \quad (107)$$

$$\rho_{Lj} = \rho(T_j, P_j, x_{ij}), \quad j = 1, 2, \ldots, 10 \quad (108)$$

$$V_j \Delta H_{VAP} - Q_R = 0, \quad j = 0 \quad (109)$$

$$V_j \Delta H_{VAP} - Q_C = 0, \quad j = 10 \quad (110)$$

$$R_{j1} = \left(\frac{MW_{Lj}}{\rho_{Lj}}\right) k_{0,1} \exp\left(-\frac{E_1}{R_g T_j}\right) x_{EOj} x_{Wj}, \quad j = 6, 7, 8, 9 \quad (111)$$

$$R_{j2} = \left(\frac{MW_{Lj}}{\rho_{Lj}}\right) k_{0,2} \exp\left(-\frac{E_2}{R_g T_j}\right) x_{EOj} x_{EGj}, \quad j = 6, 7, 8, 9 \quad (112)$$

$$K_{ij} P_j - P_{ij}^{\text{sat}} = 0, \quad j = 1, 2, \ldots, 10,\ i = 1, \ldots, N_C - 1 \quad (113)$$

$$y_{ij} - K_{ij} x_{ij} = 0, \quad j = 1, 2, \ldots, 10,\ i = 1, \ldots, N_C - 1 \quad (114)$$

$$\sum_i x_{ij} - 1 = 0, \quad \sum_i y_{ij} - 1 = 0, \quad j = 1, 2, \ldots, 10 \quad (115)$$

where $M$ is the liquid holdup, $L$ and $V$ are the liquid and vapor flows, $x$ and $y$ are the molar fractions in liquid and vapor phase, respectively, $R$ is the reaction rate, $n$ is the stoichiometric coefficient, $F$ is the feed flow rate, $z$ the feed composition, $R_g$ is the universal gas constant, $E$ is the activation energy, $T$ is the tray temperature, and $P$ is the tray pressure, $D_C$ is the column diameter, $l_W$ is the length of the weir and $h_W$ its height, $h_{OW}$ is the height of the liquid over the weir, $c_o$ is a constant, $\Delta H_{VAP}$ is the heat of vaporization,

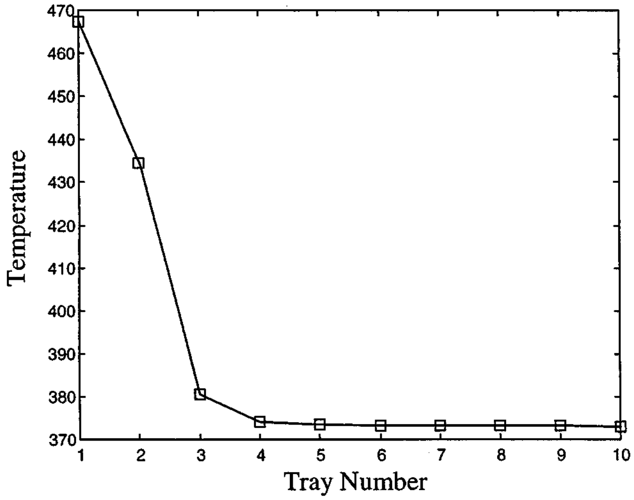


**Figure 4. Temperature profile in the reactive distillation column.**

$Q_R$ ($Q_C$) is the heat input in the reboiler (condenser), $\Delta H^R$ is the heat of reaction, $\rho_L$ is the liquid density, and $MW_L$ is the liquid molar weight. Subscript $i$ refers to the set of components (1 to $N_C$), $j$ refers to the set of trays (1 to $N_T+1$), and $k$ to the set of reactions (1 to $N_R$). All required data are obtained from Ciric and Gu (1994). In addition to the equations used by Ciric and Gu, we also use in this case study the Francis weir formula to relate the liquid outflow from a tray with the liquid holdup. An 0.083 m weir is assumed in the separation zone and a 0.166 m weir in the reaction zone. The liquid holdups are restricted between 0.01 and 0.2 m$^3$. A parametric optimization problem is solved in order to minimize the annual operating cost. The temperature profile is given in Figure 4. The feed flow rate of water and ethylene oxide are 26.314 kmol/h and 27.6 kmol/h, respectively. The heat input to the reboiler is 7.36 MW. Compared to the solution of Ciric and Gu, this solution has increased operating cost by $0.03\times10^6$ \$/yr.

The structure of the regulatory control employed is shown in Figure 3. The feed flow rate of water is used in order to set the total production rate. The feed flow rate of ethylene oxide is ratioed to the feed flow rate of water. A constant excess of 4.887% in EO is used to achieve 95% EG in the bottom product. The bottom product flow rate is adjusted to control the bottom holdup, while heat input is adjusted in order to control the product composition. The main disturbances acting on the system are the water feed flow rate (production rate level) and column pressure. The condensation rate at the top of the column is assumed to be used for controlling the column pressure. However, in order to account for the effect of the inefficiencies of this control loop, we consider the pressure variation as a major disturbance. The production rate is assumed to vary by 50% and pressure by 10% of nominal values. The problem investigated is the selection of the best tray temperature sensor location for inferential control of the EG composition at the bottom of the column. In order to mimic the ratio specification imposed on the feed flow rates of water and ethylene oxide we use the following algebraic equation

**Table 6. Reactive Distillation Column Case Study (Perfect Control)**

| | Controlled Variable | Economic Penalty (\$/yr) |
|---|---|---|
| 1 | $T_2$ | 120.90114 |
| 2 | $T_1$ | 121.18146 |
| 3 | $T_3$ | 121.53186 |
| 4 | $T_4$ | 293.19720 |

$$F_W - rF_{EO} = 0 \tag{116}$$

where $r = 1.0488$.

The perfect control formulation given by Eq. 29 is applied in order to find the best temperature sensor location for the minimization of the maximum time domain deviation of the bottom product composition in EG. The four best solutions are reported in Table 6. Controlling the temperature at tray 2 is the best solution followed by temperatures at trays 1 and 3. Then, the PI controller-based formulation is applied. The open-loop responses of the tray temperatures were fitted to first-order transfer functions and single PI controllers were designed based on the IMC tuning rules (Morari and Zafiriou, 1989). Only one detuning factor was used ($f = 1$) and one frequency $\omega = 0.1$. The results of the realistic control formulation were the same as the results of the perfect control case. This is due to the fact that Bode diagrams of all SISO loops were identical to that of a first-order system and, thus, their maximum appears at zero frequency. Since the perfect control and realistic PI control formulations are the same at zero frequency, the same structures are chosen.

In Figure 5, the closed-loop response of the bottom composition is given. In these closed-loop simulations tray temperatures are controlled using PI controllers. It is interesting to note that unstable closed-loop response is obtained by using any tray temperature above tray 3. Thus, the proposed method was successful in predicting the tray temperatures

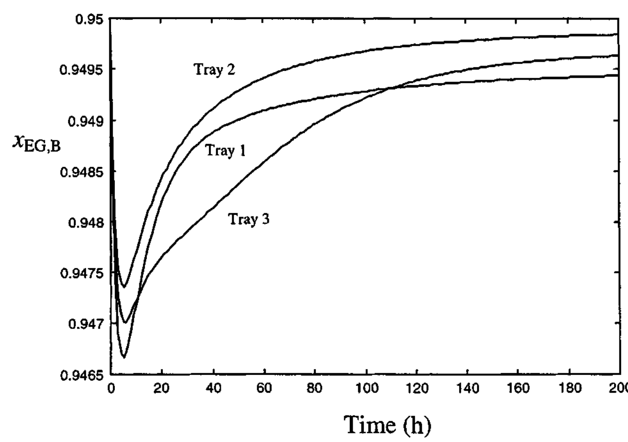


**Figure 5. Product composition response under control of different tray temperatures (reactive distillation case study).**

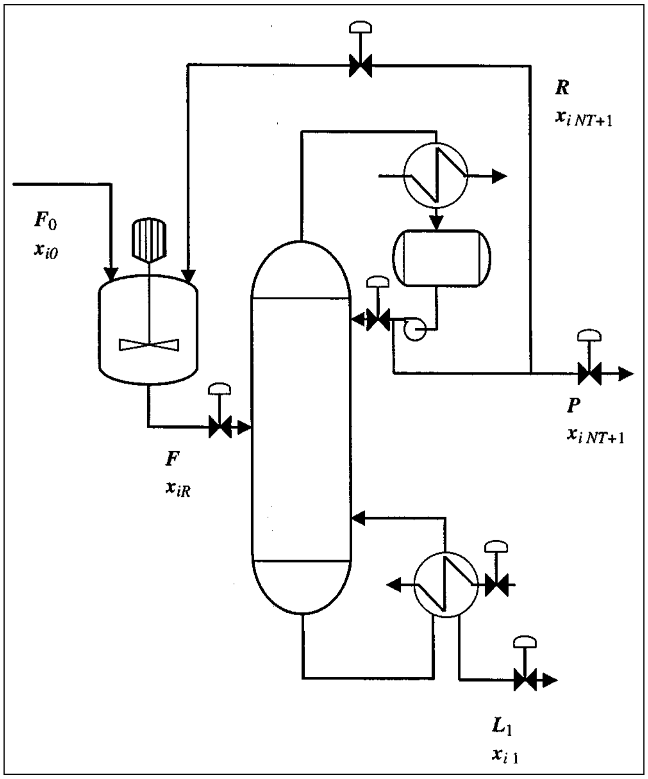


**Figure 6. Reactor/separator with recycle process.**

that should be controlled in order to minimize the variability of the product composition using an inferential control scheme.

### *Case study 3: The reactor/separator process*

The reactor/separator process is shown in Figure 6. The fresh feed consists of component A and an inert component I. The first-order irreversible reaction A $\rightarrow$ B takes place in the single-phase CSTR and transforms reactant (A) into product (B). The output of the CSTR contains all three components and is fed into a distillation column where the unreacted A is separated from the product and recycled back to the reactor. In order to avoid accumulation of the inert component in the process it is necessary to purge this material at some point. This point is mainly determined by the relative volatility of the inert. In cases where the volatility of the inert is between the volatility of reactant and product then the most plausible point is the rectifying section of the distillation column.

In order to develop a relatively simple mathematical model of the reactor/separator process the following assumptions are used

(1) The liquid on trays and in the reactor is perfectly mixed and has uniform properties.

(2) Thermodynamic equilibrium on all trays is achieved.

(3) The pressure drop in the column is negligible.

(4) Constant relative volatility and equimolar overflow.

(5) The vapor holdup is negligible.

(6) The reflux is saturated liquid.

(7) The liquid hydraulics are described by the Francis weir formula.

Then, the mathematical model of the reactor/separator process can be stated as follows

*Distillation Column* ($j = 2, 3, \ldots, NT$, $i \in \mathrm{C} = \{\mathrm{A,I}\}$)

$$\frac{d}{dt}\left(M_j x_{ij}\right) = L_{j+1}x_{ij+1} - L_j x_{ij} - V_j y_{ij} + V_{j-1}y_{ij-1} + F_j x_{iR} \tag{117}$$

$$\frac{d}{dt}\left(M_j\right) = L_{j+1} - L_j - V_j + V_{j-1} + F_j \tag{118}$$

$$y_{ij} = K_{ij}x_{ij} = \frac{\alpha_i}{\sum_{k \in C} \alpha_k x_{kj}} x_{ij} \tag{119}$$

$$V_j = V_{j-1} + (1 - q_V)F_j \tag{120}$$

$$L_j = c_o \rho_L l_W \left(h_{OWj}\right)^{3/2} \tag{121}$$

$$M_j = \left(h_W + h_{OWj}\right)\frac{\pi D_C^2}{4}\frac{\rho_L}{M_{W,L}} \tag{122}$$

$$F_j = \begin{cases} F, & j = NF \\ 0, & j \neq NF \end{cases} \tag{123}$$

*Column Base* ($j = 1$, $i \in \mathrm{C}$)

$$\frac{d}{dt}\left(M_j x_{ij}\right) = L_{j+1}x_{ij+1} - L_j x_{ij} - V_j y_{ij} \tag{124}$$

$$\frac{d}{dt}\left(M_j\right) = L_{j+1} - L_j - V_j \tag{125}$$

$$y_{ij} = K_{ij}x_{ij} = \frac{\alpha_i}{\sum_{k \in C} \alpha_k x_{kj}} x_{ij} \tag{126}$$

$$V_j = \frac{Q_R}{\Delta H^{\mathrm{VAP}}} \tag{127}$$

*Column Condenser and Reflux Drum* ($j = NT + 1$, $i \in \mathrm{C}$)

$$\frac{d}{dt}\left(M_j x_{ij}\right) = V_{j-1}y_{ij-1} - \left(L_j + P + R\right)x_{ij} \tag{128}$$

$$\frac{d}{dt}\left(M_j\right) = V_{j-1} - \left(L_j + P + R\right) \tag{129}$$

*Reactor* ($i \in \mathrm{C}$)

$$\frac{d}{dt}\left(M_R x_{iR}\right) = F_0 x_{i0} + Rx_{iNT+1} - Fx_{iR} + M_R x_{AR} n_i \kappa \tag{130}$$

$$\frac{d}{dt}\left(M_R\right) = F_0 + R - F \tag{131}$$

$$\kappa = k_0 \exp\left(\frac{-E}{R_g(T + T_0)}\right) \tag{132}$$

$$n_A = -1, \quad n_I = 0 \tag{133}$$

where $\kappa$ is the reaction rate constant. The rest of the symbols used are defined in Figure 6, as well as in the previous case study. The parameters of the model can be found in Belanger and Luyben (1998). The value of the parameter $q_V$ (heat content of the distillation feed) is set equal to one.

The open-loop response of the model is not self-regulating due to the integrating holdup dynamics in the column base, reflux drum, and reactor. In order to apply the proposed algorithm the model has to be stabilized. This is achieved by the introduction of the following algebraic equations for each of these holdups

$$L = C_V f(l)\sqrt{M} \tag{134}$$

where $L$ is the liquid outflow, $M$ is the liquid hold-up, $C_V$ is the valve constant, $f(l)$ is the flow characteristic, and $l$ is the lift.

We assume that the fresh feed consists of 95% A and 5% I. The constraints that define the feasible operation of the process are summarized below

$$g_1 = 239.5 - L_1 \leq 0 \tag{135}$$

$$g_2 = M_1 - 100 \leq 0 \tag{136}$$

$$g_3 = 30 - M_1 \leq 0 \tag{137}$$

$$g_4 = M_{NT+1} - 250 \leq 0 \tag{138}$$

$$g_5 = 100 - M_{NT+1} \leq 0 \tag{139}$$

$$g_6 = M_R - 3{,}000 \leq 0 \tag{140}$$

$$g_7 = 1{,}000 - M_R \leq 0 \tag{141}$$

$$g_8 = V_{NF} - 1{,}200 \leq 0 \tag{142}$$

$$g_9 = 400 - V_{NF} \leq 0 \tag{143}$$

$$g_{10} = R - 400 \leq 0 \tag{144}$$

$$g_{11} = -R \leq 0 \tag{145}$$

$$g_{12} = 0.9895 - x_{1,B} \leq 0 \tag{146}$$

Constraint $g_1$ assures that the production rate will be greater than the minimum acceptable. Constraints $g_2$ to $g_7$ are related to minimum and maximum holdup levels, while constraints $g_8$ and $g_9$ are related to flooding and weeping constraints. Constraints $g_{10}$ and $g_{11}$ are related to the maximum rate of recycle that can be achieved. Finally, constraint $g_{12}$ is a product purity constraint.

The objective function to be maximized is the value of the products minus the cost of utilities and raw material

$$J = \left(0.10 \cdot L_1 - 0.05 F_0 - 250 \frac{5}{10^6} \cdot V_1\right) \cdot 8{,}760 \cdot 50, \text{ in \$/yr} \tag{147}$$

The effective degrees of freedom for the optimization are the potential manipulated variables

$$u = [\, L_1 \; V_1 \; L_{NT+1} \; R \; P \; F \,]^T \tag{148}$$

The optimum value of the objective function is 4.955 $10^6$ \$/year. The values of the optimization variables at the solution are

$$u = \begin{bmatrix} L_1 \\ V_1 \\ L_{NT+1} \\ R \\ P \\ F \end{bmatrix} = \begin{bmatrix} 298.611 \\ 901.389 \\ 652.916 \\ 198.661 \\ 49.813 \\ 547.084 \end{bmatrix} \tag{149}$$

Constraints $g_6$ and $g_{12}$ are active at the optimum solution.

The perfect control formulation for control structure selection was applied to the reactor/separator process. To this end, the following potential controlled variables and disturbances are selected

$$y = \begin{bmatrix} x_{B,1} \\ x_{A,NT+1} \\ x_{I,NT+1} \\ M_1 \\ M_{NT+1} \\ M_R \\ x_{A,R} \\ x_{I,R} \end{bmatrix}, \quad p = \begin{bmatrix} F_0 \\ x_{A,0} \\ q_V \end{bmatrix} \tag{150}$$

In Table 7 the results of the application of the perfect control formulation are summarized. The magnitudes of the disturbance vector elements was equal to 5% of their nominal values. The most promising structures are the ones that control all holdups and composition of the product in the column bottom. The column bottoms flow rate, the purge flow rate, and reactor outflow are included as manipulated variables in the most promising structures. Controlling the compositions in the reactor or in the recycle stream is not necessary for this system. Furthermore, the system exhibits high sensitivity to the magnitude of the disturbance in the fresh feed flow rate and composition. These conclusions are in close agreement with those of Belanger and Luyben (1998) (structure I2 in their article).

Finally, it was assumed that no composition measurements are available for the distillation column system. In this case inferential composition control is an alternative strategy. Tray temperatures at selected locations are controlled in order to

**Table 7. Reactor/Separator Case Study (Direct Composition Control)**

| Rank | Manipulated Variables | Controlled Variables |
|---|---|---|
| 1 | $L_1, P, V_1, F$ | $M_D, M_B, M_R, x_{B,1}$ |
| | $L_1, P, L_{NT+1}, F$ | $M_D, M_B, M_R, x_{B,1}$ |
| 2 | $L_1, P, L_{NT+1}, R$ | $M_D, M_B, M_R, x_{B,1}$ |
| | $L_1, P, V_1, F$ | $M_D, M_B, M_R, x_{B,1}$ |
| | $L_1, P, R, F$ | $M_D, M_B, M_R, x_{B,1}$ |
| 3 | $L_1, P, L_{NT+1}, F$ | $M_D, M_B, M_R, x_{A,NT+1}$ |
| 4 | $L_1, P, L_{NT+1}, R$ | $M_D, M_B, M_R, x_{A,NT+1}$ |
| 5 | $L_1, P, R, F$ | $M_D, M_B, M_R, x_{A,NT+1}$ |
| 6 | $L_1, P, V_1, F$ | $M_D, M_B, M_R, x_{A,NT+1}$ |
| 7 | $L_1, P, V_1, R$ | $M_D, M_B, M_R, x_{A,NT+1}$ |

Table 8. Best Structures for the Reactor/Separator Case Study (No Direct Composition Control)

| | Manipulated Variables | Controlled Variables |
|---|---|---|
| One point control | $L_1$, $L_{NT+1}$, $P$, $R$ | $M_D$, $M_B$, $M_R$, $T_4$ |
| Two point control | $L_1$, $L_{NT+1}$, $V_1$, $P$, $R$ | $M_D$, $M_B$, $M_R$, $T_4$, $T_{22}$ |

reduce the variability of the product composition. The potential measurements are the following

$$y = \begin{bmatrix} T_2 \\ \vdots \\ T_{NT} \\ M_1 \\ M_{NT+1} \\ M_R \\ x_{A,R} \\ x_{I,R} \end{bmatrix}, \quad p = \begin{bmatrix} F_0 \\ x_{A,0} \\ q_V \end{bmatrix} \tag{151}$$

that is, tray temperatures are included in the measurement vector instead of composition measurements. In this case the control structure is defined by the value of 40 binary variables, and the number of alternatives is extremely large ($2^{40}$). Two cases are examined. In the first case one point composition control is assumed. The algorithm converges after the examination of 15 control structures requiring only a few minutes of cpu time. The optimum structure is given in Table 8. In the second case two point control is assumed and the algorithm converges after the examination of 29 alternative control structures. The results are also given in Table 8. It is interesting to note that even in the case where direct composition control is not available, the reactor composition is not selected as controlled variable in the best control structures. Furthermore, the control of a tray temperature close to the column bottoms seems to be an effective means for composition control.

Finally, the MILP formulation that uses decentralized PI control was applied. SISO PI tunings were obtained, as in the previous case studies. Two detuning factors per input-output pair were considered, namely $f = 0.25$ and $f = 1$. A 5% variation of the disturbances was assumed. It is interesting to note that the number of alternatives in this case study is extremely large. A simple application of Eq. 67 shows that this number equals to 3.04 $10^6$. The best control structure corresponds to the following $\Xi$ matrix

$$\Xi = \begin{bmatrix} 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \end{bmatrix} \tag{152}$$

This matrix corresponds to the control structure selected as the best solution when perfect control was used (see Table 7). Heat input at the reboiler is used in order to control bottoms composition. Product flow rate, purge flow rate, and reactor outflow are used to control columns bottom level, reflux drum level, and reactor level, correspondingly. In addition the detuning factor $f = 1$ was selected in all loops. In Figures 7 and 8 the closed loop system response to a 20% change in production level (set by fresh feed flowrate) and 5% change in fresh feed composition is shown. The closed loop dynamics of this system, as can be seen from these figures, is acceptable. Although we cannot claim that this is the best closed loop structure for this system the proposed method identified a structure that can control the system effectively.

## Conclusions

The choice of suitable sets of manipulated and controlled variables as well as their interconnection is a challenging problem. A modification of the previous work of Narraway and Perkins (1993) on this problem is presented in this article. The control objectives are posed in terms of economic penalties associated with the effect of disturbances on key process variables. These control objectives are then related

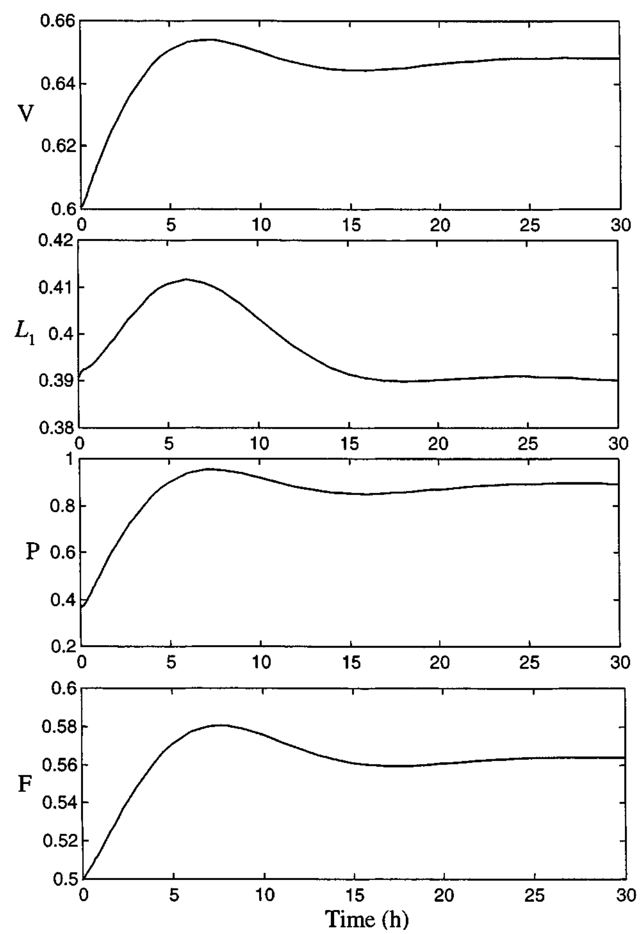


**Figure 7. Closed-loop response of the reactor/separator system-manipulated variables.**

20% change in production rate and 5% change in feed composition.

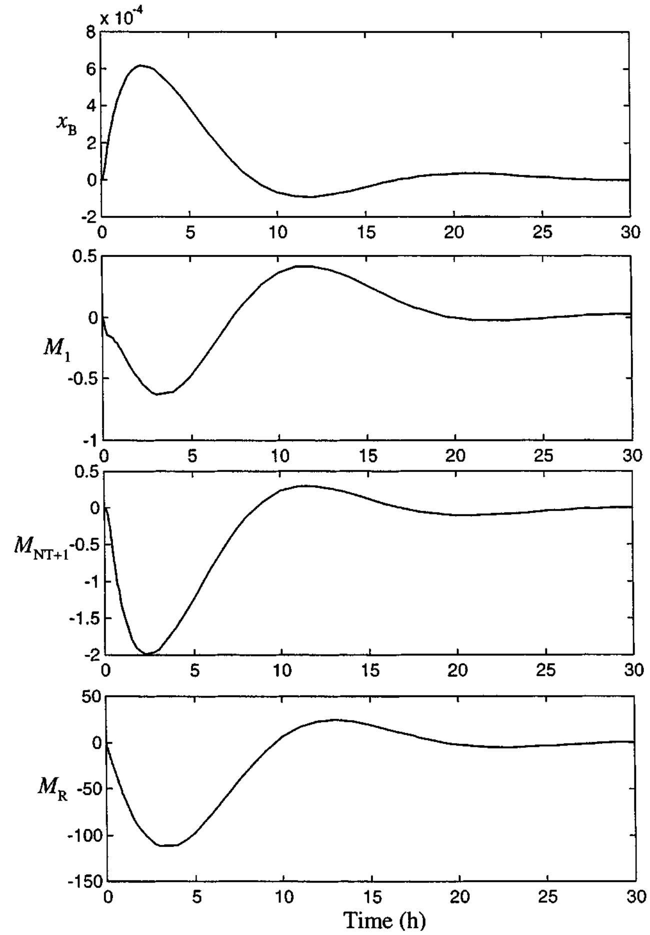


**Figure 8. Closed-loop response of the reactor/separator system-controlled variables.**

20% change in production rate and 5% change in feed composition.

to a subset of the potential measured variables, and a suitable set of control variables is selected among the potential manipulated variables so that the dynamic economics is as favorable as possible. Two control algorithms, perfect control and realistic, decentralized PI control, have been included in the formulation for the examination of the closed-loop system. Integer variables are used to model these control algorithms resulting in an MINLP formulation of special structure. By exploiting its structure, the problem is transformed into an MILP problem that can be solved effectively avoiding the need for complete enumeration of all alternatives. At the same time, global optimality is guaranteed. Application of this approach to a number of case studies demonstrates that the method can effectively be used in order to answer important questions arising in the control structure selection problem.

## Notation

$f$ = discrete detuning factor
$f_s$ = scaling factor used in Eq. 13
$\mathbf{h}$ = vector of equality constraints
$I$ = identity matrix of dimension equal to the dimension of the vector given as subscript
$j = \sqrt{-1}$
$n$ = length of the vector used as a subscript ($n_y$ equals the length of vector $y$)
$p$ = index over the set of periods
$P$ = Laplace transform of the $p$ vector
$p$ = vector of disturbances
$s$ = complex variable
$t$ = time
$U$ = Laplace transform of the $u$ vector
$W$ = vector of binary variables that select the set of manipulated variables
$X$ = Laplace transform of the $x$ vector
$y$ = vector of the potential measurements
$Y$ = Laplace transform of the $y$ vector
$Z$ = vector of binary variables that select the set of controlled variables

### Greek letters

$\alpha$ = gradient of the cost function with respect to the state variables
$\beta$ = gradient of the cost function with respect to the input variables
$\delta$ = deviation variable
$\mathbf{\Lambda}$ = relative gain array
$\lambda$ = Lagrange multipliers
$\rho$ = linear estimate of the back-off vector
$\Sigma$ = Laplace transform of the $\sigma$ vector
$\sigma$ = linear estimate of the deviation of the inequality constraints from their nominal values
$\omega$ = frequency

### Subscripts

0 = initial conditions
$A$ = algebraic variable
$cl$ = closed loop
$D$ = differential variable
$H$ = maximum allowable variation
$L$ = lower bound
$U$ = upper bound

### Superscripts

$I$ = imaginary part or integral variable
MIMO = multi-input, multi-output system
$R$ = real part
SISO = single-input, single-output system

## Literature Cited

Bahri, P. A., A. Bandoni, and J. Romagnoli, "Operability Assessment in Chemical Plants," *Comput. Chem. Eng.*, **20**, S1787 (1996).
Belanger, P. W, and W. L. Luyben, "Plantwide Design and Control of Processes with Inerts. 3. Intermediate Inerts," *Ind. Eng. Chem. Res.*, **37**, 535 (1998).
Brenan, K. E., S. L. Campbell, and L. R. Petzold, *Numerical Solution of Initial Value Problem in Differential-Algebraic Equations,* North-Holland, New York (1989).
Buckley, P. S., *Techniques of Process Control,* Wiley, New York (1964).
Campo, P. J., and M. Morari, "Achievable Closed-Loop Properties of Systems Under Decentralized Control: Conditions Involving the Steady-State Gain," *IEEE Trans. Autom. Control.*, **39**, 932 (1994).
Ciric, A. R., and D. Gu, "Synthesis of Nonequilibrium Reactive Distillation Processes by MINLP Optimization," *AIChE J.*, **40**, 1479 (1994).
Dimitriadis, V. D., and E. N. Pistikopoulos, "Flexibility Analysis of Dynamic Systems," *Ind. Eng. Chem. Res.*, **34**, 4451 (1995).
Figueroa, J. L., P. A. Bahri, A. Bandoni, and J. Romagnoli, "Economic Impact of Disturbances and Uncertain Parameters in Chemical Processes—a Dynamic Back-Off Analysis," *Comput. Chem. Eng.*, **20**, 453 (1996).

Georgiou, A., and C. Floudas, ''Structural Analysis and Synthesis of Feasible Control Systems—Theory and Applications,'' *Chem. Eng. Res. & Des.*, **67**, 600 (1989).
Glover, F., ''Improved Linear Integer Programming Formulations of Nonlinear Integer Problems,'' *Manage. Sci.*, **22**, 455 (1975).
Heath, J., J. D. Perkins, and S. Walsh, ''Control Structure Selection based on Linear Dynamic Economics—Multiloop PI Structures for Multiple Disturbances,'' *Proc. IFAC World Cong.*, San Francisco, **M**, 85 (1996).
Lee, W., and V. W. Weekman, ''Advanced Control Practice in the Chemical Process Industry: A View from Industry,'' *AIChE J.*, **22**, 27 (1976).
Luyben, M., and C. Floudas, ''A Multiobjective Optimisation Approach for Analysing the Interaction of Design and Control,'' *Interactions Between Process Design and Process Control*, J. D. Perkins, ed., Pergamon, Oxford, p. 101 (1992).
Luyben, W. L., *Process Modelling Simulation and Control for Chemical Engineers*, McGraw Hill, New York (1990).
Luyben, W., B. Tyreus, and M. Luyben, *Plantwide Process Control*, McGraw Hill, New York (1999).
Maarleveld, A., and J. E. Rijnsdorp, ''Constraint Control of Distillation Columns,'' *Automatica*, **6**, 51 (1970).
Marlin, T. E., *Process Control, Designing Processes and Control Systems for Dynamic Performance*, McGraw Hill International Editions, New York (1995).
Mohideen M. J., J. D. Perkins, and E. N. Pistikopoulos, ''Optimal Design of Dynamic Systems under Uncertainty,'' *AIChE J.*, **42**, 2251 (1996).
Moore, C., ''Selection of Controlled and Manipulated Variables,'' *Practical Distillation Control*, W. L. Luyben, ed., Van Nostrand Reinhold, NY (1992).
Morari, M., and E. Zafiriou, *Robust Process Control*, Prentice Hall, Englewood Cliffs, NJ (1989).
Morari, M., and J. D. Perkins, ''Design for Operations,'' *Int. Conf. on Foundations of Computer-Aided Process Design*, L. T. Biegler and M. F. Doherty, eds., CACHE-AIChE Publications (1995).
Narraway, L. T., J. D. Perkins, and G. W. Barton, ''Interaction between Process Design and Process Control: Economic Analysis of Process Dynamics,'' *J. of Process Control*, **1**, 243 (1991).
Narraway, L. T., and J. D. Perkins, ''Selection of Process Control Structures Based on Linear Dynamic Economics,'' *Ind. Eng. Chem. Res.*, **32**, 2681 (1993).
Narraway L. T., and J. D. Perkins, ''Selection of Process Control Structure Based on Economics,'' *Comput. Chem. Eng.*, **18**, S511 (1994).
Newell, R. B., and P. L. Lee, *Applied Process Control— A Case Study*, Prentice-Hall, Sydney (1989).
Nishida, N., G. Stephanopoulos, and A. W. Westerberg, ''A Review of Process Synthesis,'' *AIChE J.*, **27**, 321 (1981).
Owen, P. S., ''Control Structure Selection Based on Economics and Linear Multivariable Controllers,'' Transfer Report, Imperial College, Univ. of London, London, U.K. (1996).
Perkins, J. D., ''Interactions Between Process Design and Process Control,'' *DYCORD+ 1989 Proceedings*, Maastricht, The Netherlands (1989).
Perkins, J. D., and S. Walsh, ''Optimisation as a Tool for Design/Control Integration,'' *Comput. Chem. Eng.*, **20**, 315 (1996).
Rijnsdorp, J. E., ''Chemical Process Systems and Automatic Control,'' *Chem. Eng. Prog.*, **63**, 97 (1967).
Stephanopoulos, G., ''Synthesis of Control Systems for Chemical Plants: A Challenge for Creativity,'' *Comput. Chem. Eng.*, **7**, 331 (1983).
Turkay, M., T. Gurkan, and C. Ozgen, ''Synthesis of Regulatory Control Structures for a Styrene Plant,'' *Comput. Chem. Eng.*, **17**, 601 (1993).
Wang, F. Y., and I. T. Cameron, ''Control Studies on a Model Evaporation Process—Constrained State Driving with Conventional and Higher Relative Degree Systems,'' *J. of Process Control*, **4**, 59 (1994).
Williams, H. P., *Model Building in Mathematical Programming*, 2nd ed., Wiley, New York (1985).

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