Effect of Disturbances in Optimizing Control: Steady-State Open-Loop Backoff Problem

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One of the key components in the operation of chemical plants is the ability to operate over a range of conditions while satisfying performance specifications. A method for determining the necessary open-loop backoff from a steady-state nominal optimum is introduced to ensure that disturbances cause no constraint violation. This approach consists of defining a joint optimization-flexibility problem that can be solved within an optimization framework based on an iterative procedure. By formulating the optimization problem in economic terms, the backoff in the objective function is a measurement of the open-loop economic penalty that is necessary to be paid to achieve feasible operation over the disturbance range of interest (considering the worst combination). An upper bound on the economic potential available for closed-loop control can then be established, providing a valid reference for ranking different control schemes. Three examples presented illustrate the application of this approach: (1) a simple linear example, (2) a system of two CSTRs; and (3) an industrial distillation column.

Introduction

In recent years the modern processes have become more difficult to operate because of the trend toward larger, more highly integrated plants with smaller surge capacities between various processing units. Such plants give the operations little opportunity to prevent upsets from propagating from one unit to another interconnected unit. In view of the increased emphasis on safe, efficient plant operation, it is only natural that the subject of process control has become increasingly important in the last three decades. In fact, without process control it would not be possible to operate most modern processes safely and profitably, while satisfying plant quality standards. Therefore considerable incentive exists to apply controls to processes lacking them, to improve the control of those already being regulated, and *to find the proper operating conditions and set points of the controlled plant that guarantee the* economic performance, *and certainly its* operability.

Therefore a good process design must exhibit operability characteristics that will allow economic performance to be realizable in a practical operating environment. This requires the plant to operate feasibly over a variety of operating conditions (flexibility), and to have a good dynamic performance, as well as the ability to deal effectively with disturbances (controllability). So there is a need for an approach to consider both these issues in the operation of a chemical plant (with a proposed design). In this article, we seek a method that enables us to calculate a figure of merit for two measuring purposes:

1. Controllability to rank alternative control strategies
2. Flexibility to guarantee the feasible plant operation

with the objective being a measure of the economic performance of the plant. The starting platform to attack this problem is the open-loop case (no control), from which the upper bound on the cost of the controller and the penalty associated with the economic performance of the plant in the absence of process control will be defined. This can also be used as a tool to analyze how much benefit can be provided by advanced control implementation.

For the steady-state open-loop case, that is, the one considered in this article, the problem has the following characteristics: A process is under steady-state operation without or with minimum control action on it (open loop) at a point determined by optimizing the process for some nominal value of the uncertain parameters. In this situation it is difficult to

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get feasible operation when the values of the uncertain parameters change. Then we would like to find another operating point, if any exists at all, that remains feasible under the presence of disturbances without demanding any control action, and that requires the minimum deviation from the current best nominal operation of the plant. By finding this point, which from now on will be called the backoff point, we would be able to set the economic penalty that is necessary to be paid in order to prevent infeasible operation, without having a control system installed. *On the other hand, this economic penalty can be seen as an estimation of the maximum amount of money that is worth being spent in a control system if we decide to install it. Furthermore, this provides a way to rank different controllers from the point of view of how much of the amount lost because of the backoff can be recovered.*

The steady-state open-loop backoff calculation for a plant with fixed design leads to the problem of flexibility in operation. From a practical point of view, a distinction should be made between the problem of flexibility in design and our approach of flexibility in operation. In the design problem the process plant itself does not exist yet, and despite an attempt to simultaneously consider uncertainty by adjusting design and control (operating) variables, the emphasis is on finding a feasible design of minimum capital cost. Our approach of flexibility in operation, on the other hand, is related more to the issue of controlling the process, where something must be done to reject the disturbances on a continuous operation base. Notwithstanding these practical differences, the mathematical formulations of both problems are closely related; it poses the problem of flexibility in operation as a particular case of the flexibility in design, where the design variables remain fixed. For this reason, the natural way addressing the rigorous mathematical treatment of these problems has been accomplished by developing a mathematical procedure for flexibility in design and by extending it to the problem of flexibility in operation.

Many attempts have been made during the past 15 years to deal with different aspects of the flexibility problems. These vary in approach, solution strategies, and scope of applicability. Broadly speaking, two major approaches could be distinguished: stochastic and deterministic. The first approach is based on the assumption of some kind of probabilistic distribution of the parametric uncertainties, while the deterministic approach tries to set in advance some realization of the uncertain parameters or simply assume that every single realization has the same probability. The deterministic approach demands less information about the uncertain parameters than the stochastic approach. Simply, it is required to know an average (or best known) value and an estimated range of variation for each single parameter subject to uncertainty. This is also the most common situation in real applications, where it is very unusual to obtain extra information about the uncertainties or disturbances. For this reason the approach has proved to be very practical in real application.

Grossmann and Halemane (1982, 1983) were among the first to present a mathematical formulation for the problem of design under uncertainty. Their approach has been successively improved to overcome problems such as infinite dimensionality and the assumption of vertex solution for the worst case of the constraints (Grossmann and Floudas, 1987). Several other algorithms have been presented for special cases, such as using the linear model of the process (Pistikopoulos and Grossmann, 1988; Bandoni and Romagnoli, 1989). These last authors used a different approach, through an iterative cutting plane algorithm, extending the procedure of Friedman and Reklaitis (1975). In this case the coefficients of the model matrix and the independent terms were considered not necessarily uncertain on their own, but their uncertainty stems from their functional dependence on some parameters that are in turn subject to uncertainty.

Following the work of Bandoni and Romagnoli (1989), a new approach was used here to calculate the amount of steady-state open-loop backoff from the nominal optimum operating point of a chemical plant (with fixed design) to estimate the effect of disturbances on the process operation.

The article is organized as follows: the next section presents the general problem of steady-state open-loop optimization of the operation of a process plant and the effect of disturbances. In the third section the formulation of the open-loop back-off problem is given. The mathematical algorithm is presented in the fourth section, where the linear and nonlinear cases, the similarities and differences between this approach and the existing methodologies, and some convergence properties are also discussed. In the fifth section, three case studies, ranging from a simple linear problem to an industrial problem, are presented. Finally, in the sixth section, the conclusions and future works are given.

Steady-State Optimization Problem

The ultimate goal in well-operated chemical plants is to achieve optimum plant performance (such as economic profit, controllability, and safety) within the various limitations place on plant operation. Typically, the steady-state optimization is performed by determining optimum operating conditions that maximize (or minimize) an appropriate objective function, subject to the process model (a set of equality constraints) and operational restrictions (inequality contraints). The process parameters are usually fixed at some nominal (average or best known) values.

The typical steady-state open-loop optimization problem of an existing process can be stated in the following form:

$$\min \Phi\left(z, x, \theta^N, p_p\right)$$

subject to

$$\begin{aligned} h_i\left(z, x, \theta^N, p_p\right) &= 0 \qquad i \in E \\ g_j\left(z, x, \theta^N, p_p\right) &\le 0 \qquad j \in I \\ z &\in Z, \end{aligned} \tag{1}$$

where $z \in Z = \{z : z^L \le z \le z^U\}$ is a vector of control (independent) variables, x is a vector of state (dependent) variables, θ^N is a vector of nominal values of the process uncertainties, and p_p is the vector of process parameters; E and I are the set of indexes of equality and inequality constraints, respectively; the equations h_i represent the mathematical model of the process, involving mass and energy balances,

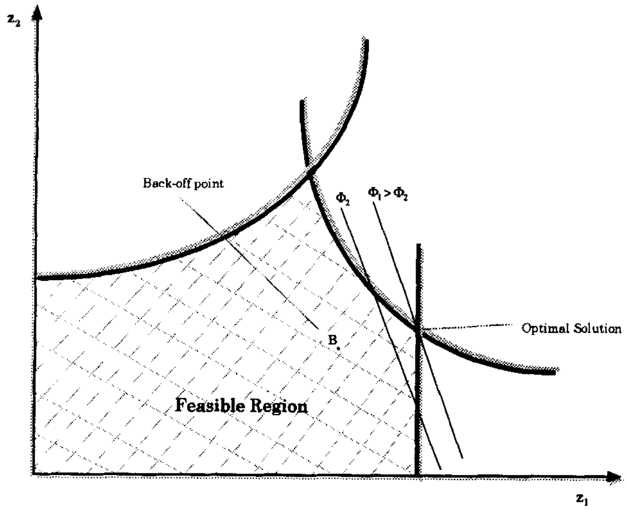

Figure 1. Typical operating window.

equipment performance relationships, and so forth; and the inequalities g_j are the process limitations in terms of raw materials, unit capacities, product qualities, and so forth.

The constraints play a crucial role in the optimization of chemical processes. Usually, the optimum operating condition of an industrial plant is determined by a subset of these constraints acting as active constraints. This situation can be visualized for a very simple example (only two independent variables) in Figure 1, where the shape of the objective function contours and constraints are such that the optimum operating point is completely determined by the two active constraints C_1 and C_2. A constrained optimum is by far the most common situation in the process industry. This is because the high complexity of the plants, with a large number of interacting variables and tight physical and economical limitations, as well as safety regulations, invariably leaves the unconstrained optimum of the objective function outside the feasible operating region (Arkun and Stephanopoulos, 1980; Marleveld and Rijnsdorp, 1970).

Effect of disturbances on optimal operation

Most of the time, a process will be subject to some kinds of disturbances. The whole concept of optimizing control is based on the relative time scales of typical disturbances in comparison to the response time of the plant. This suggests a classification of those disturbances into "slow" and "fast." The slow disturbances may be handled by an on-line, or even off-line optimizer, while the fast disturbances must be managed by a regulation system, whose aim is to hold the plant at the desired (optimum) steady-state point. In this article we are interested in the fast disturbances and how to deal with them to get feasible operation while minimizing the amount lost.

The effect of fast disturbance at the regulation level is to perturb the plant from a desired steady state, which may lead to constraint violation. To avoid this situation, despite the disturbances, the operating point should be moved away from that determined by the optimization level, as requiring the steady state to be precisely on the active constraints will result in infeasible operation. We will refer to the extent of this movement of the operating point due to the likely effect of disturbances as *backoff*. In Figure 1, point B represents the backoff position. The backoff point belongs to the permanent feasible region (PFR), the region within which the plant will always operate feasibly, even in the face of disturbances or uncertainties. Using the concept of PFR in the flexibility analysis of a chemical plant is quite useful, since its size can be used as a qualitative measure of the flexibility of the plant.

Without a previous analysis of the effects of the disturbances on the process, it is not possible to determine in advance how large this movement should be, if any movement is actually required, to avoid constraint violations. From this point of view, it is interesting to establish first the effect of disturbances at steady state, when no control action is taken (i.e., the open-loop case). This effect is a property of process and disturbances only (Narraway et al., 1991). By comparing the values of objective function at the nominal optimum and the backoff point, one can easily establish an upper bound on the amount lost in the performance criteria that is necessary to incur in order to guarantee open-loop feasibility. If the objective function is given in economic terms (profit, cost, etc.), this penalty directly provides an upper bound on the amount of money that should be spent on a control system, in order to minimize the process variability (and consequently the amount lost) close to the steady-state active constraints. Therefore, by using the concepts of backoff and PFR, it can be shown that the implementation of a control system may completely change the results of steady-state flexibility analysis, since *the flexibility is not only an inherent quality of the process design and operating conditions, but also depends on the selected control systems and configuration.*

Open-Loop Backoff Calculation

Problem formulation

In order to apply the mathematical results and numerical techniques of optimization theory to concrete engineering problems, it is necessary to clearly delineate the boundaries of the engineering system to be optimized, to define the quantitative criterion on the basis of which candidates will be ranked to determine the "best," to select the system variables that will be used to characterize or identify candidates, and to define a model that will express the manner in which the variables are related. This composite activity constitutes the process of problem formulation that is perhaps the most crucial step in any problem that involves optimization.

As mentioned before, in this work the concept of backoff is used for the steady-state flexibility analysis of a chemical plant. Since the ultimate goal is to calculate the amount of the backoff for a closed-loop system (i.e., with control), the method to be used should have the following specifications:

- The process dynamics can easily be accommodated within this methodology, and there should not be much problem in solving the resulting dynamic flexibility problems.
- Because of the earlier case, the strategy used for flexibility analysis should be as simple as possible (at least of the same order of difficulty as the nominal optimization of the plant). This is also true for the steady-state flexibility analysis of real applications, where there is not much room for assumptions or simplifications, and the simulation of the plant is contained in a dedicated program (black box) or must be built with commercial simulators.

• The strategy can be used for simultaneous controllability and flexibility analysis, as well as for design or retrofit design purposes.

The approach used in this article is based on these lines of reasoning. It consists of an iterative procedure that can be solved within any optimization framework. Here, in order to characterize the necessary open-loop backoff, the region of variation for disturbances should be defined first. This definition depends on the type of information about the disturbances that is available. There are two aspects that would need to be known about the uncertain parameters: probability of occurrence and dynamics. If some kind of probability distribution of the occurrence of each single disturbance is available, the stochastic approach, as outlined in the first section, could be used. Even in this case, the dynamics of the disturbances entering the system should be set or known in order to outline a procedure to reject them. The difficulty with this, in industrial problems, is that it is very difficult to obtain enough records of each single process disturbance in order to establish their probability distributions or dynamics.

As indicated in the first section, the most typical situation is known as the nominal, best-known, or average value for each disturbance and an estimation of its range of change. In this work we assume that only this information is available, and therefore a region Γ containing all the possible realizations of the disturbances can be defined as

$$\Gamma = \{\boldsymbol{\theta}:\boldsymbol{\theta}^L \le \boldsymbol{\theta} \le \boldsymbol{\theta}^U\}. \tag{2}$$

Furthermore, if in the absence of better information, a uniform distribution for the disturbances realization is assumed, any choice of $\boldsymbol{\theta} \in \Gamma$ is equally probable. Since $\boldsymbol{\theta}$ is a parameter in the functions describing the process constraints, each single realization $\boldsymbol{\theta}^k \in \Gamma$ will result in a different set of constraints, and then a different feasible region will be generated. The corresponding region F^k can be expressed as

$$F^k = F\left(z, \boldsymbol{x}, \boldsymbol{\theta}^k, \boldsymbol{p}_p\right) = \left\{z:h_i\left(z, \boldsymbol{x}, \boldsymbol{\theta}^k, \boldsymbol{p}_p\right) = 0, g_j\left(z, \boldsymbol{x}, \boldsymbol{\theta}^k, \boldsymbol{p}_p\right) \le 0, z \in Z, i \in E, j \in I\right\}. \tag{3}$$

Clearly, $F^N = F(z, \boldsymbol{x}, \boldsymbol{\theta}^N, \boldsymbol{p}_p)$ is the original region with the nominal value of disturbances, $\boldsymbol{\theta}^N$. From Eq. 3, the "flexibility" due to uncertainty in the value of disturbances may then be introduced into the original optimization problem Eq. 1 in order to define the following steady-state open-loop optimization problem with flexibility:

$$\min \Phi\left(z, \boldsymbol{x}, \boldsymbol{\theta}^N, \boldsymbol{p}_p\right) \tag{4}$$

subject to

$$h_i\left(z, \boldsymbol{x}, \boldsymbol{\theta}^k, \boldsymbol{p}_p\right) = 0 \qquad i \in E$$
$$\max_{\boldsymbol{\theta} \in \Gamma} \max_{j} g_j(z, \boldsymbol{x}, \boldsymbol{\theta}, \boldsymbol{p}_p) \le 0 \qquad j \in I$$
$$z \in Z$$
$$\boldsymbol{\theta}^k \in \Gamma.$$

Due to the uniform distributions assumed for disturbances, any $\boldsymbol{\theta}^k \in \Gamma$ is equally probable, therefore Eq. 4 will have an infinite number of constraints, resulting in a "semi-infinite" optimization problem.

Algorithm Development

The solution of the semi-infinite programming problem, Eq. 4, is particularly difficult. The algorithm proposed below is based on a simple decomposition into two levels of optimization problem. The first level (outer level (OL)) seeks the *optimality* of Eq. 4 for a fixed disturbances vector, while the second level (inner level (IL)) tests its *feasibility* under different realizations of the disturbances, looking at each single constraint one at a time. This is done in an iterative procedure until an *optimal* and *feasible* solution for any disturbance is found, provided that such a solution exists.

Assuming that z^* is the optimal solution of Eq. 4, the procedure to find it can be stated as

$$\text{find } z^*: z^* \text{ gives the minimum of } \boldsymbol{\Phi}\left(z, \boldsymbol{x}, \boldsymbol{\theta}^N, \boldsymbol{p}_p\right) \tag{5a}$$
$$\forall \boldsymbol{\theta}^k \in \Gamma, z^* \in F^k, \tag{5b}$$

where F^k is defined in Eq. 3. This condition can be guaranteed if we are able to characterize a region of feasibility H such that, for any $z^* \in H$, Eq. (5b) is verified. Region H can be established based on the concept of *worst case* with respect to the disturbances, for each single constraint. This is normally a very conservative point of view, but it provides the only means of safety guaranteeing there is no constraint violation. Region H can be generated in an iterative procedure, starting from the nominal region F^N and removing those portions that do not verify Eq. 5b. In this sense, the procedure outlined below is like a cutting plane algorithm, where the cuts are given by nonlinear surfaces instead of planes.

Assume $z^{*(n)}$ to be the optimal vector corresponding to the nth iteration of the algorithm (to be proposed later). For each constraint, the worst case of the disturbances around this point, $z^{*(n)}$, corresponds to the vector $\boldsymbol{\theta}$ that results from the optimal solution of the following optimization problem for $j \in I$:

$$\max g_j\left(z^{*(n)}, \boldsymbol{x}, \boldsymbol{\theta}, \boldsymbol{p}_p\right) \tag{6}$$

subject to

$$h_i\left(z^{*(n)}, \boldsymbol{x}, \boldsymbol{\theta}, \boldsymbol{p}_p\right) = 0 \qquad i \in E$$
$$\boldsymbol{\theta} \in \Gamma.$$

Let $\boldsymbol{\theta}^{k(n)}$ be the vector $\boldsymbol{\theta}$ that satisfies Eq. 6 for $k \in I$ at iteration n. If $g_k(z^{*(n)}, \boldsymbol{x}, \boldsymbol{\theta}^{k(n)}, \boldsymbol{p}_p) \ge 0$, the constraint is violated and then the corresponding index k is included in the set $K^{(n)}$ defined as: $K^{(n)} = \{k$:k is the index corresponding to a violate constraint$\}$. Each different $\boldsymbol{\theta}^{k(n)}$ from Eq. 6 generates a feasible region $F^{k(n)} = F(z, \boldsymbol{x}, \boldsymbol{\theta}^{k(n)}, \boldsymbol{p}_p)$. Then at each iteration of the algorithm, a region $F^{(n)}$, which is the intersection of all the regions generated by the vectors $\boldsymbol{\theta}^{k(n)}$ of that iteration, can be defined as: $F^{(n)} = \cap F^{k(n)}$ for $k \in K^{(n)}$. Finally, the region $H^{(n)}$ containing all the regions generated until the current iteration n can be defined as: $H^{(n)} = F^{(n)} \cap H^{(n-1)}$, where $H^{(0)} = F^N$. Note that the following sequence holds: $H^{(0)} \supseteq H^{(1)} \supseteq H^{(2)} \supseteq \cdots H^{(n-1)} \supseteq H^{(n)}$.

Assuming that the last region $H^{(n)}$ is not empty, the optimality can be incorporated into the problem in each iteration if the z^* vector used in Eq. 6 is found through the following optimization problem:

$$\min \Phi\left(z, x, \theta^N, p_p\right) \tag{7}$$

subject to

$$z \in H^{(n)}.$$

The final region $H^{(n)}$ is called the *permanent feasible region* (PFR), the region within which, despite the effect of all disturbances $\theta \in \Gamma$, the plant will operate feasibly.

Based on the preceding ideas, an algorithmic procedure for solving the steady-state open-loop backoff problem is given as follows:

Step 1. Solve Eq. 1 to obtain the nominal optimal solution (with nominal values of disturbances) z^{*N}.

Step 2. Set $n = 1$, $z^{*(0)} = z^{*N}$ and $K^{(0)} = \{k{:}k = j \in I,\}$.

Step 3. Solve Eq. 6 for $j \in I$, to generate the perturbations $\theta^{k(n)}$.

Step 4. Check feasibility. If $z^{*(n)}$ verifies all constraints (g_j) for $j \in I$, within a given tolerance, END. Otherwise update $K^{(n)}$ and continue.

Step 5. Solve Eq. 7 for $z^{*(n)}$.

Step 6. Set $n = n + 1$ and go back to Step 3.

Note that in Step 3 of the algorithm it is necessary to solve $j \in I$ different optimization problems. This may be very tedious if the original problem, Eq. 1, has a large number of inequality constraints. But it is important to note that, in a typical industrial problem, the number of inequality constraints is normally not very large, particularly if compared with the number of equality constraints.

Another remark on the preceding algorithm is that one can easily incorporate a dropping constraint scheme by removing the constraints that are no longer violated from the set $K^{(n)}$. Another aspect of the IL subproblems for Eq. 6 is that they are very similar in different iterations. Actually, through the iterations, the structure of IL problems remains the same, and only the objective function changes in the value of a constant, the vector $z^{*(n)}$. This is the main reason why this algorithm normally converges in a few iterations, usually between 2 and 4 (from our computational experience). Moreover, the optimum vector $\theta^{k(n)}$ found in iteration n is a good initial guess for the same problem at the next iteration.

Figures 2a and 2b show a diagram of the outer and inner level subproblems for each iteration of the steady-state open-loop backoff calculation algorithm. It should be noticed that each of these subproblems can be posed as a nonlinear programming (NLP) optimization problem.

Comparison between this approach and existing methods

One of the approaches in steady-state flexibility analysis that is similar to the one presented in this article is algorithm II in Halemane and Grossmann (1983). In that algorithm,

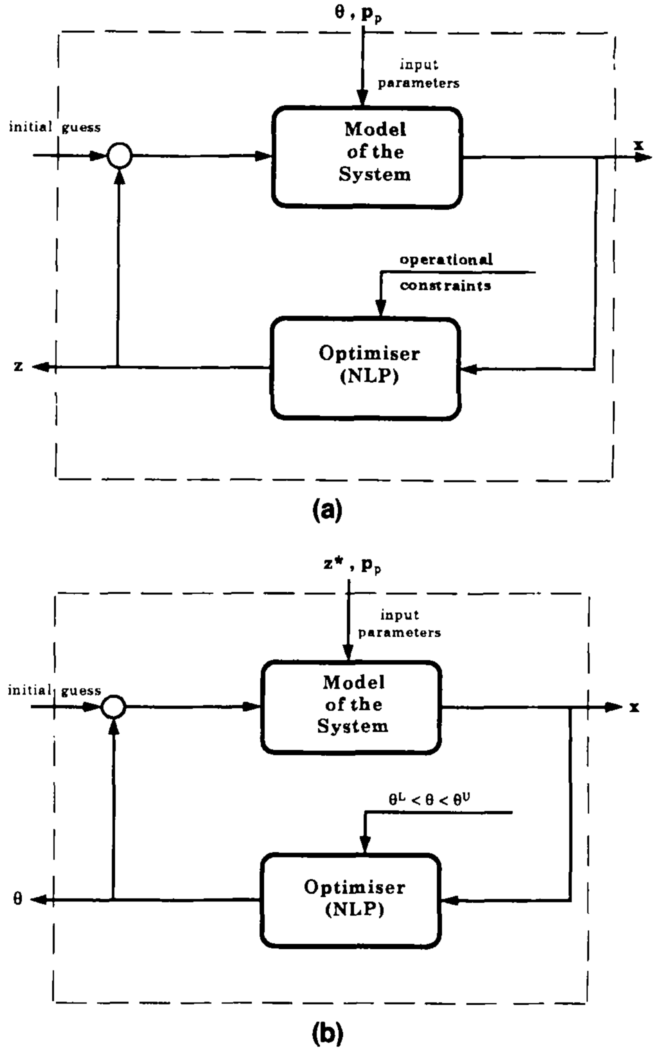

Figure 2. (a) Outer and (b) inner levels in backoff calculation algorithm.

given the uncertainty parameter set $T = \{\theta \mid \theta^L \le \theta \le \theta^U\}$, the *feasibility test* for a design consists of ensuring that for every $\theta \in T$, there exists a control variable z that can be selected during plant operation to satisfy each one of the constraint functions f_j, $j \in J$. This step is formulated as

$$\chi(d) = \max_{\theta \in T} \min_{z} \max_{j \in J} f_j(d, z, \theta).$$

The solution θ^c of this problem defines a critical point for feasible operation. Halemane and Grossmann assume that these critical points correspond to vertices or extreme values. Therefore, their approach does require exhaustive vertex searches. The algorithm presented in this article starts with only one critical point (nominal disturbances), but their algorithm requires an initial set of uncertainty parameters. They find the initial set by the method proposed by Grossmann and Sargent (1978). It should be noticed that although critical θ values are frequently at vertices, we cannot always be sure about it, and later Grossmann and Floudas (1987) proposed another approach to eliminate this assumption.

Another similar approach is the one proposed by Grossmann and Floudas (1987), which is the feasibility test (or actually the inner-loop subproblem in our algorithm) for the case when there are no control variables. Actually, the feasibility test in our algorithm is the same as this one. But it should be noted that the approach given by Grossmann and Floudas consists of the feasibility test of a process, while our approach is a complete flexibility analysis of a chemical plant.

One major difference between our approach and most of the existing methodologies for flexibility analysis is that we consider the control variables to be constant during the plant operation. The reason for this assumption comes from several factors, such as:

- It is very difficult, if not impossible, to have on-line measurements of some of the input disturbances (e.g., concentration), most of the uncertain parameters (e.g., heat transfer coefficient, catalyst activity, etc.), and model uncertainties. Therefore, manipulation of control variables due to these changes are not possible.
- For the constant manipulation of control variables due to uncertainties, an on-line optimizer is needed to find the optimal conditions. Therefore, the control variables should be fixed during the period of each optimization run (which may take a few hours for large plants).

Therefore, in these situations, considering the possibility for continuous manipulation of control variables can lead to serious overestimation of the inherent flexibility of a process.

Convergence considerations

To guarantee the convergence of the algorithm to a permanent feasible solution (PFS), global optimums for Eqs. 6 and 7 are required. From Eq. 7 to provide the best solution over the PFR and from Eq. 6, in order to ensure that the worst case of each constraint is obtained and consequently the last region $H^{(n)}$ is really the permanent feasible one, for any disturbances $\theta \in \Gamma$. To analyze the convergence of the algorithm, let's have a look at the two different cases that may arise, according to the form of Eq. 1.

Nonlinear Case. If any of the equations involved in Eq. 4 is not linear, the problem will be an NLP problem. Consequently, the problem must verify the conditions for global optimization. Such conditions are very strong and quite often do not occur in practical applications. Horst and Tuy (1993) give a review of different strategies to find the global optimum. For certain problems with a given structure, there are theoretical approaches for global optimization as mentioned in Horst and Tuy. For the general case, a practical technique that can be applied is the so-called "multistart technique," which consists of selecting different starting points using either a deterministic grid or a random sampling. In the first case, the feasibility region is subdivided into separate sectors and the optimization is carried out in each of them. In the second case, a random number generator can be used, and the feasibility of the constraints will be checked using each of the selected points.

Linear Case. If the functions used in the equations are all linear, Eq. 4 will be linear too. Consequently, the complete algorithm can be solved using standard linear programs (LPs), and the corresponding solutions of Eqs. 6 and 7 are global solutions. Therefore the convergence to a PFR in a finite number of steps can be guaranteed. This can be established on the basis that any optimal solution to an LP problem must be a basic feasible solution, and there is a finite number of them. This means that after a finite number of iterations, the solutions of Eqs. 6 will start to be repeated and then no extra constraint will be added to the OL subproblems and the algorithm stops (Bandoni and Romagnoli, 1989).

First-order approximation

Most methodologies for process-control design have been developed based on linear process representations, so having them available we can use an alternative approach for estimating the open-loop backoff, that is, through a first-order estimation based on these linear models. In this case, the conditions of the linear case in the previous section are verified and the convergence to a PFR can be guaranteed.

A first-order estimation of the size of the backoff in the absence of control can be determined considering a linear transfer function model relating inputs ($\boldsymbol{u}$) and disturbances ($\boldsymbol{\theta}$) to the chosen output variables ($\boldsymbol{y}$):

$$\boldsymbol{y}(s) = \boldsymbol{G}(s)\cdot\boldsymbol{u}(s) + \boldsymbol{G}_d(s)\cdot\boldsymbol{\theta}(s). \tag{8}$$

Here, using similar arguments as in the previous section for the estimation of the size of the movement away from the optimum, a new optimization problem based on the steady-state linearized model of the process can be defined. The problem is stated as

$$\max \Phi(\boldsymbol{u}, \boldsymbol{y}, \boldsymbol{\theta}^N) \tag{9}$$

subject to

$$\begin{aligned} &\boldsymbol{y} = \boldsymbol{G}(0)\cdot\boldsymbol{u} + \boldsymbol{G}_d(0)\cdot\boldsymbol{\theta} \\ &\boldsymbol{u}^L \le \boldsymbol{u} \le \boldsymbol{u}^U \\ &\boldsymbol{y}^L \le \boldsymbol{y} \le \boldsymbol{y}^U \\ &\boldsymbol{\theta} \in \Gamma. \end{aligned}$$

Just as before, different feasible regions, which in this case are defined as, $F(\boldsymbol{u}, \boldsymbol{y}, \boldsymbol{d}) = \{\boldsymbol{u}: \boldsymbol{y} = \boldsymbol{G}(0)\cdot\boldsymbol{u} + \boldsymbol{G}_d(0)\cdot\boldsymbol{\theta}, \boldsymbol{u}^L \le \boldsymbol{u} \le \boldsymbol{u}^U, \boldsymbol{y}^L \le \boldsymbol{y} \le \boldsymbol{y}^U\}$, will be generated for any choice of $\boldsymbol{\theta} \in \Gamma$.

Obviously, Eq. 9 can be solved using the algorithm presented in the fourth section.

Case Studies

The methodology for backoff calculation discussed in the previous sections will be evaluated within the context of three examples. The first example is a simple linear optimization problem, with one independent variable and one disturbance. The second example is a flowsheet consisting of two continuous stirred tank reactors (CSTRs) in series with an intermediate mixer. This example has two independent variables and two disturbances. Here we can graphically reproduce the different regions and show how the algorithm proceeds. The third one is the application of the backoff calculation procedure to an industrial distillation column, which shows that this methodology can be implemented into real plants. All these processes have been simulated in the SPEEDUP flowsheeting package (1993), and both the SPEEDUP and GAMS (Brooke et al., 1992) packages have been used for the solution of the different optimization problems.

Example 1

Since the global convergence to the PFR for a linear process is guaranteed, as the first example let us consider a simple linear system in which two inputs u_1 and u_2 affect a state variable x that is measured as the output y. The system is modeled by a first-order differential equation as follows:

$$\frac{dx}{dt} = 3u_1 + 4u_2 - x + d$$
$$y = x,$$

or in terms of transfer functions:

$$y(s) = \frac{3}{s+1}u_1 + \frac{4}{s+1}u_2 + \frac{1}{s+1}d.$$

The optimization problem is posed as "maximizing the profit while operating within the input and output constraints and satisfying the steady-state model equation":

$$\max \Phi = -5u_1 - 6u_2 + 7y$$

subject to

$$y \le 10$$
$$u_1 \ge 10$$
$$u_2 \ge 0$$
$$y = 3u_1 + 4u_2 + d.$$

The nominal value and upper bound for the disturbance, d, are given as: d:[0, 3]. By solving the preceding optimization problem, using u_1 and u_2 as decision variables, the first two constraints become active and the variables u_1 and u_2 will have the values 0 and 2.5, respectively.

The steady-state open-loop backoff calculation algorithm has been applied to this example. Figure 3 shows the original operating window and also the permanent feasible regions for this system. The summary of the progress of the procedure is as follows:

Iteration 1. (a) Step 1: gives the optimum P_1 over the feasible region R_1

(b) Steps 3 and 4: first constraint is violated, the region R_2 is determined with the worst case of this constraint.

Iteration 2. (a) Step 1: gives the optimum P_2 over the feasible region R_1 and R_2

(b) Steps 3 and 4: no constraint is violated, the algorithm stops.

Point P_2 is the permanent feasible point (PFP) that belongs to the PFR. At this point the decision variables and objective function have the values $u_1 = 0$, $u_2 = 1.75$, and $\Phi = 38.5$, so there is a 30% reduction betwee.ı the objective function values of nominal optimum and backoff points. Therefore, by using some kind of controllers, we can recover most of the loss in the objective value.

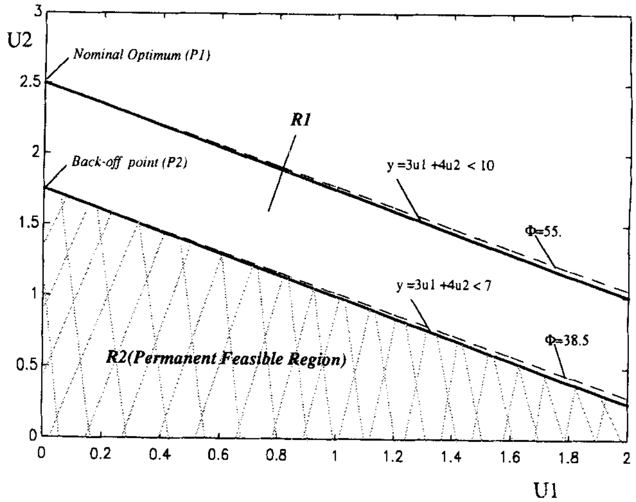

Figure 3. Nominal and permanent feasible regions for the linear process.

Example 2

Consider the flowsheet of Figure 4 taken from de Hennin and Perkins (1991). It consists of a system of two CSTRs in series with an intermediate mixer introducing the second feed. A single, irreversible, exothermic, first-order reaction ($A \rightarrow B$) takes place in both reactors. Details of the model equations representing the material and energy balances can be found in the report. The model has two degrees of freedom, and the eight inequality constraints considered are:

C_1: $T^1 \le 350$,	C_2: $T^2 \le 350$,
C_3: $Q_F^1 + Q_F^2 \le 0.8$,	C_4: $\text{Cool}^1 \le 30$,
C_5: $\text{Cool}^2 \le 20$,	C_6: $Q_F^1 \ge 0.05$,
C_7: $Q_F^2 \ge 0.05$,	C_8: $C^2 \le 0.3$.

The objective function (Φ) used in the optimization problem is related to the net profitability of the flowsheet. Both feed flowrates, Q_F^1 and Q_F^2, are used as the optimization (decision) variables.

For this study we considered two possible disturbances given by the temperature and composition of the feeds to the reactors, T_F and C_F. The lower bounds, nominal values, and upper bounds are given below:

T_F (K):	(298, 300, 315)
C_F (mol/m^3):	(19.5, 20, 21).

For the nominal disturbances, the optimum point is at the intersection of constraints 1 and 5 (this means that the nomi-

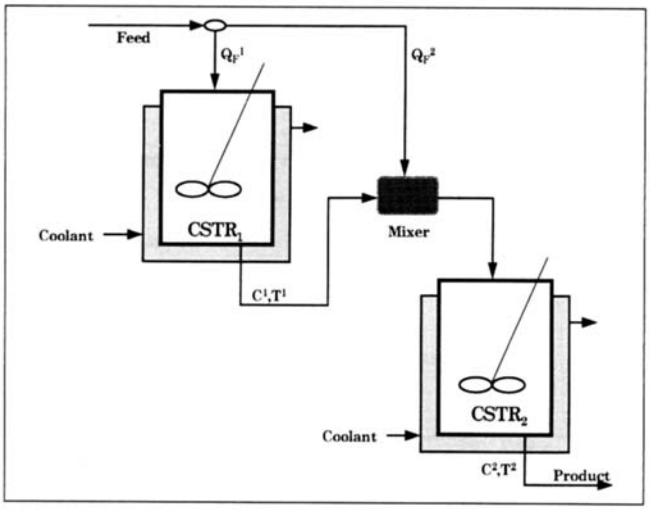

Figure 4. Flowsheet example (two CSTRs + mixer).

nal problem is fully constrained, as the number of active constraints is equal to the number of decision variables). The optimum solution is

$$\Phi = 90.3522\ \$/\text{h}$$

$$Q_F^1 = 0.3552\ \text{m}^3/\text{s}$$

$$Q_F^2 = 0.2062\ \text{m}^3/\text{s}.$$

The nominal operating window is shown in Figure 5. As can be seen, the region is nonconvex and the objective-function-level curves are nonlinear functions. Despite this situation, it can be seen on the figure that the preceding solution is the global optimal solution. The multistart method (as discussed in the previous section) has also been used for this example, to search for the global optimum.

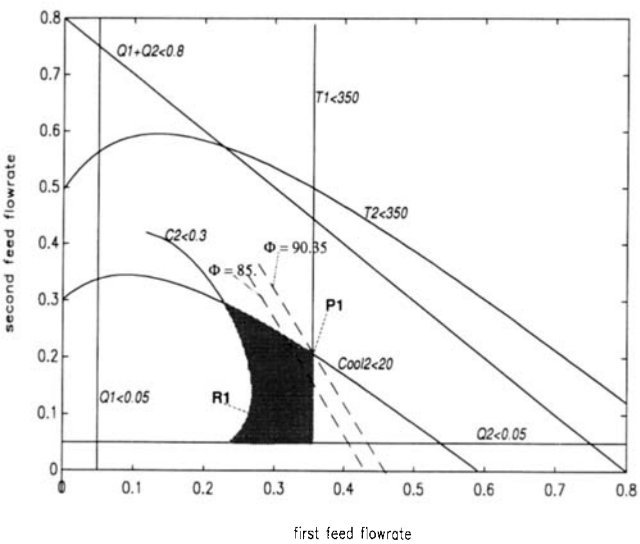

Figure 5. Nominal operating window for two CSTRs example.

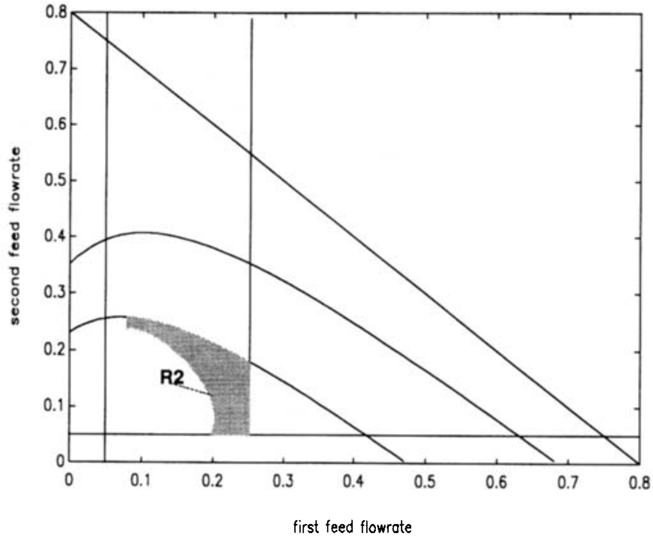

Figure 6. Movement of operating window for disturbances: $T_F = 315$, $C_F = 21$.

The algorithm described before was used to calculate the steady-state open-loop backoff for this flowsheet. Figures 6 and 7 show the movement of the original operating window due to the disturbance combinations found in the inner loops of the first and second interations of the backoff algorithm. The disturbance combinations determined by the inner loops are as follows:

Iteration 1: $T_F\,(\text{K}) = 315$, $\quad C_F\,(\text{mol/m}^3) = 21$,

Iteration 2: $T_F\,(\text{K}) = 298$, $\quad C_F\,(\text{mol/m}^3) = 19.5$.

A summary of the progress of the algorithm is given below:

Iteration 1. (a) Step 1: gives the optimum P_1 over the feasible region R_1 (Figure 5)

(b) Steps 3 and 4: constraints C_1 and C_5 are violated, the region R_2 is determined by the worst case of each constraint.

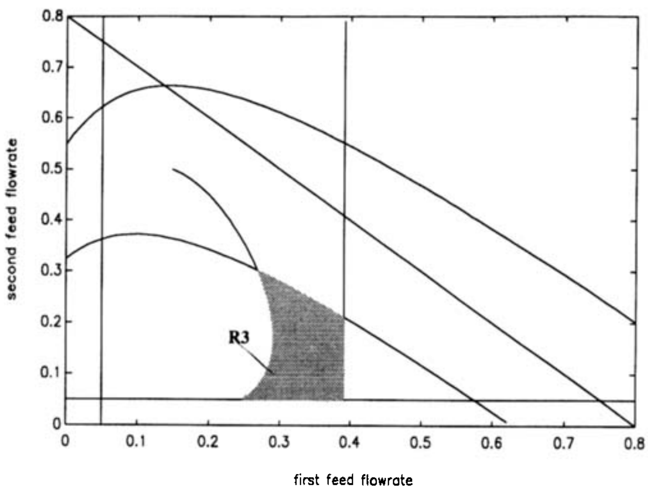

Figure 7. Movement of operating window for disturbances: $T_F = 298$, $C_F = 19.5$.

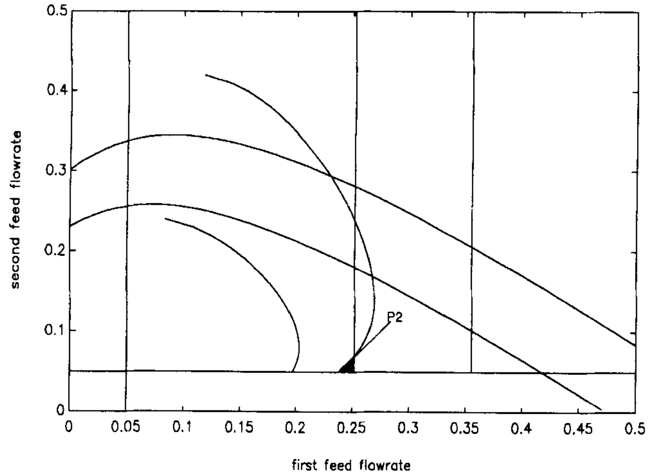

Figure 8. Feasible region found in the second-iteration outer loop (two CSTRs example).

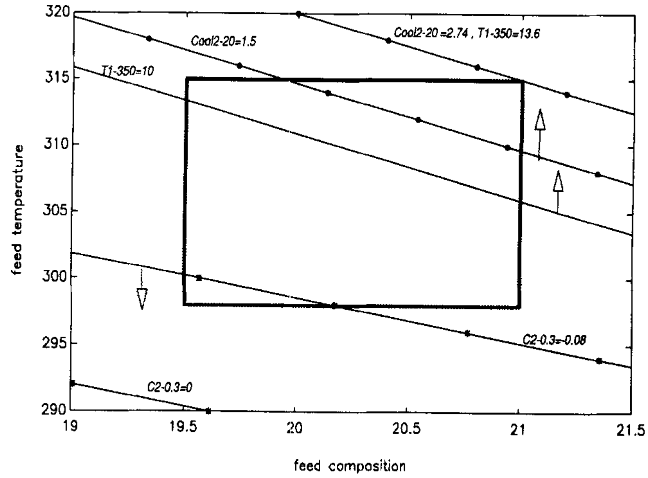

Figure 10. Operating region for the inner-level subproblem of first iteration (two CSTRs example).

Iteration 2. (a) Step 1: gives the optimum P_2 over the regions R_1 and R_2 (Figure 8)

(b) Steps 3 and 4: constraint C_8 is violated, the region R_3 is determined as before.

Iteration 3. (a) Step 1: gives the optimum P_3 over the regions R_1, R_2, and R_3 (Figure 9)

(b) Steps 3 and 4: no constraint is violated, so the algorithm stops.

Figures 8 and 9 show the feasible regions found in the outer loops (Step 1) of the second and third iterations (the feasible region for the outer loop of the first iteration is actually the nominal operating window shown in Figure 5). The permanent feasible region is actually the intersection of regions R_1, R_2, and R_3 (Figure 9). Figures 10 and 11 give the operating regions for the inner-level subproblems of iterations 1 and 2, respectively. As can be seen from the figures, these regions are completely convex; therefore, the global optimality of the inner loops is guaranteed.

Table 1 gives the number of decision variables and objective functions found from the outer levels (Step 1) of each of these iterations. The final point, P_3, is the PFP (permanent feasible point) over the PFR of the system. Therefore, in light of the given disturbances, in order to guarantee the open-loop feasible operation of this system, it is necessary to set the operating point at (0.252, 0.055) instead of at the original point (0.355, 0.206). This means a reduction of 48% in the nominal objective function. For this particular example there is a large incentive to install a control system that is capable of recovering as much as possible of the 48% loss in profit.

Example 3

The third case study here is a large industrial column used to produce high-purity propylene (> 99.5%), which is required for polymer production (see Figure 12). The main disturbances affecting this column are feed flow rate, feed composition, and the wet-bulb temperature of the ambient air

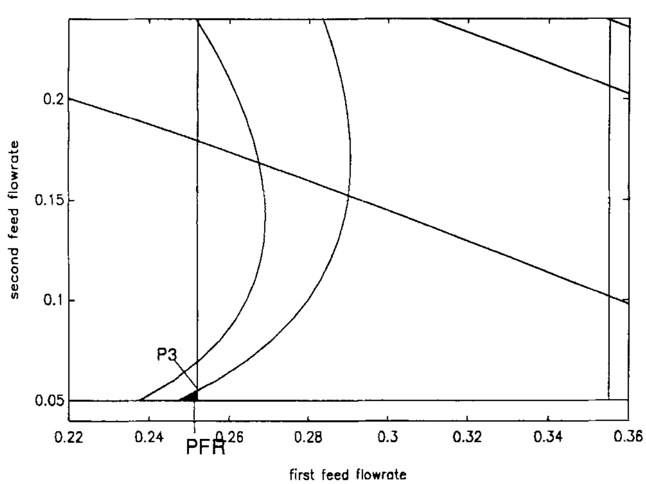

Figure 9. Feasible region found in the third-iteration outer loop (two CSTRs example).

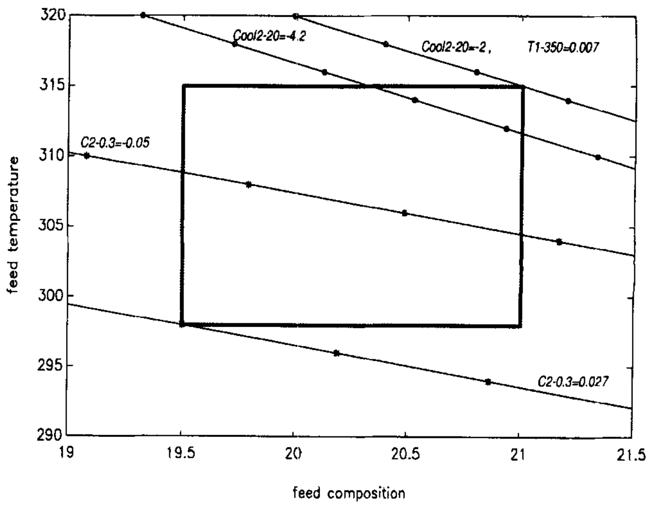

Figure 11. Operating region for the inner-level subproblem of second iteration (two CSTRs example).

Table 1. Values for Decision Variables and Objective Function in Each Iteration: Two CSTRs + Mixer

	Iter.	Q_F^1	Q_F^2	Φ
Point P1	1	0.355	0.206	90.35
Point P2	2	0.252	0.069	49.12
Point P3	3	0.252	0.055	46.86

(affecting the performance of the cooling tower). To investigate its operation, a compartmental-type dynamic model of this column developed by Lear (1992), and implemented in SPEEDUP, has been used. The column's operation is constrained by the following, with the objective of producing the maximum amount of polymer-grade propylene (PGP):

(a) Maximum column pressure (≤ 1.62 MPa)

(b) Maximum acceptable product propane impurity (≤ 0.006 mol fraction)

(c) Minimum acceptable bottom product composition (≥ 0.75 mol fraction)

(d) Maximum available reboiler heat (≤ 18 MW)

(e) Maximum cooling water flow rate (≤ 29 kmol/s)

The optimization variables used to find the optimal operation of this column are:

(a) Product flow rate

(b) Vent flow rate

(c) Reboiler heat input

(d) Cooling water flow rate

With these variables and nominal values of disturbances, the optimum point was found using the steady-state version of the model. At this point, three operating parameters (pressure, propane impurity in the distillate, amount of cooling in the condenser) were at their maximum allowable limits. Figure 13 shows the nominal feasible region for this column.

To analyze the effect of the disturbances in this system the bounds on the disturbances should be defined first. The lower, nominal, and upper bound values (with respect to the real data from the plant) are as follows:

Feed rate: (5.0, 5.5, 6.5 kmol/min)

Feed composition: (0.13, 0.165, 0.18 mol % propane)

Wet-bulb temperature: (278, 293, 298 K).

After using the backoff calculation algorithm, the PFP will be found within two iterations. In Figure 13, the position of the backoff point (PFP) is shown. It should be noticed that, since the third decision variable (cooling water flow rate) is always at its maximum value, to get Figure 13, the feasible region is given with the rest of the optimization variables.

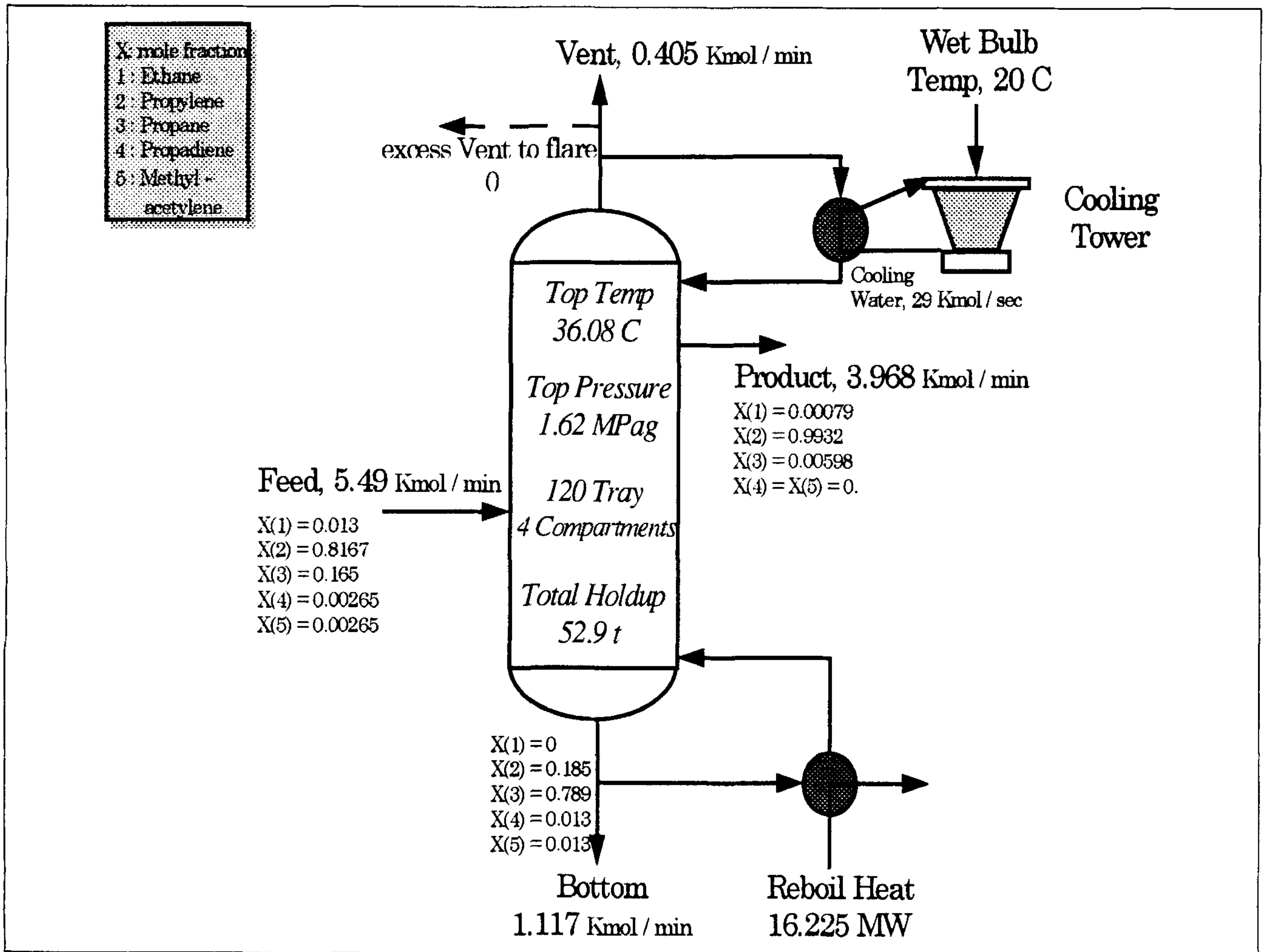

Figure 12. Industrial distillation column.

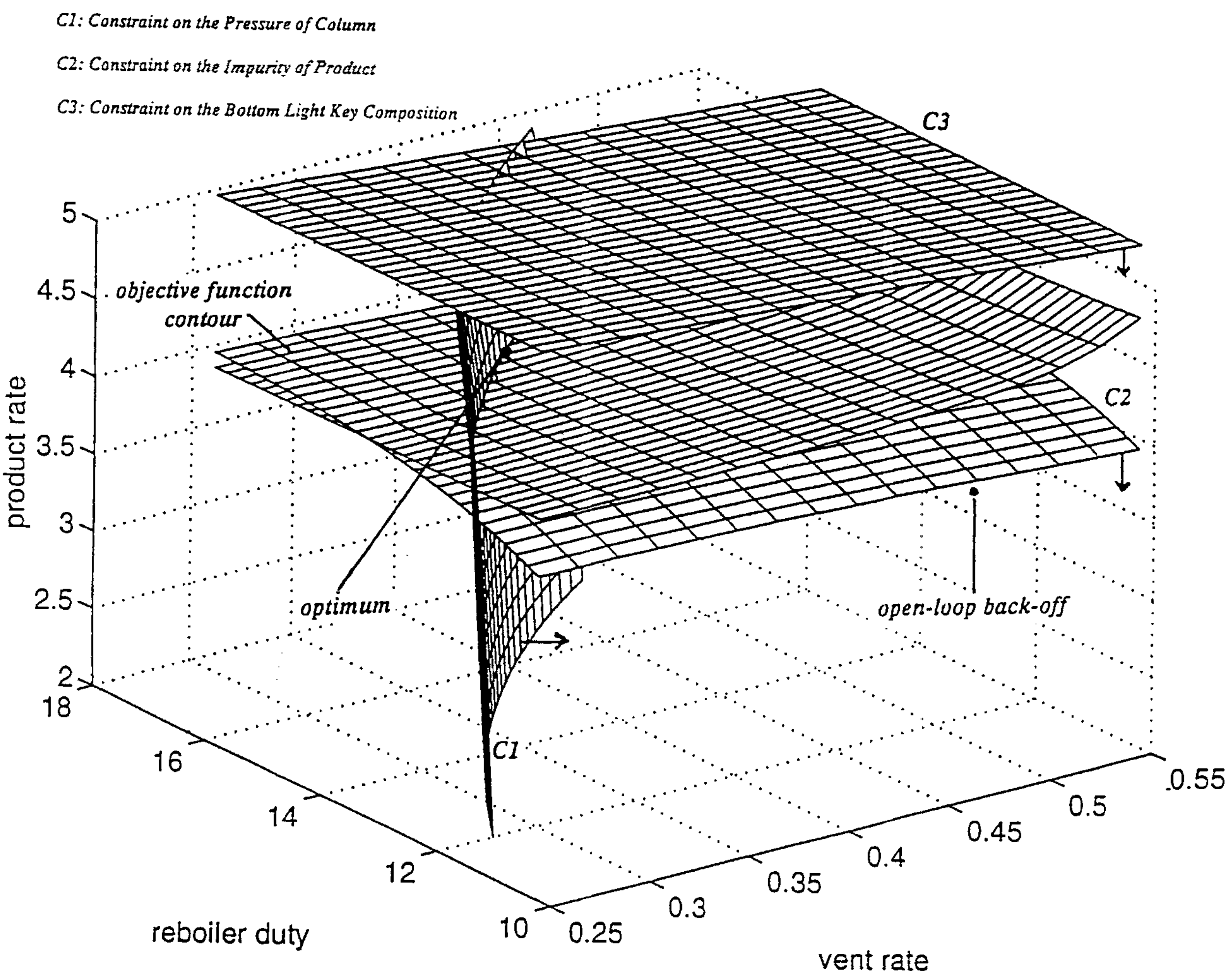

Figure 13. Nominal operating window, and the position of optimum and backoff points for distillation column.

From this figure we can also see that the feasible region is convex, so the global optimality can be easily achieved. A summary of the progress of the algorithm is given below:

Iteration 1. (a) Step 1: gives optimum P_1 over the feasible region R_1.

(b) Steps 3 and 4: Constraints 1 and 2 are violated. The two new operating windows R_2 and R_3 are determined for the worst case of each of these constraints.

Iteration 2. (a) Step 1: gives optimum P_2 over the feasible regions R_1, R_2, and R_3.

(b) Steps 3 and 4: no constraint is violated, so the algorithm stops.

Figure 14 gives the operating window for the inner level (Steps 3 and 4) of the first iteration. As can be seen, the region and the different objective function contours are quite convex, so the global convergence is guaranteed. It should be noticed that in the inner loop, two different combinations of disturbances caused the violation of constraints 1 and 2. These combinations are given below:

First combination:	feed flow rate = 5.0; feed composition = 0.18; wet-bulb temperature = 298.
Second combination:	feed flow rate = 6.5; feed composition = 0.13; wet-bulb temperature = 298.

The amount of decision variables and objective functions found in the outer loops (Step 1) of the backoff calculation iterations are given in Table 2. The final point, P_2 (found in the second iteration), is the permanent feasible point, and it

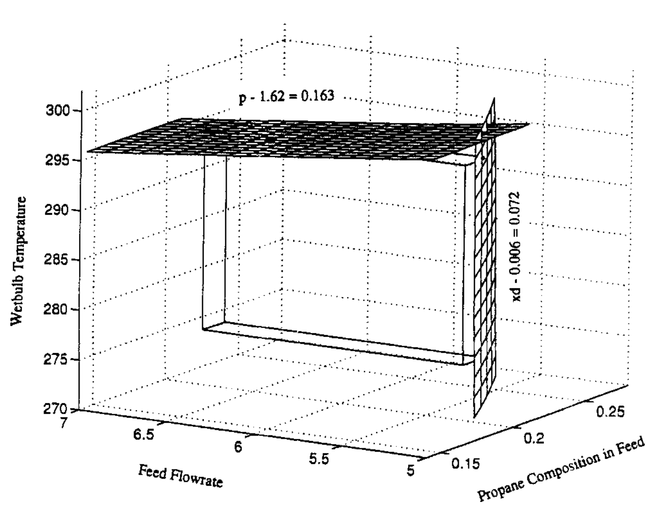

Figure 14. Operating region for the inner-level subproblem of first iteration (distillation column).

Table 2. Values of Optimization Variables and Objective Function in Backoff Algorithm: Distillation Column

	Iter.	Product Flow Rate	Vent Flow Rate	Reboiler Heat Input	Cooling water Flow Rate	Objective Function
Point P1	1	3.968	0.405	16.225	29	87.931
Point P2	2	3.257	0.550	13.771	29	72.360

is necessary to move to this backoff point to guarantee the open-loop feasible operation, which means a reduction of 17.7% in the objective function relative to the nominal value. Consequently, for this particular example, again there is a strong incentive to install a high-performance control system that would allow us to recover as much as possible of the loss in profit. According to current prices, in this specific situation, the penalty due to backoff from the optimum point is of the order of 800,000 Australian dollars per year. The next step is to investigate how much of this penalty can be recovered using different controllers.

Conclusions

A methodology to calculate the steady-state open-loop backoff has been presented. This is implemented within an optimization framework and has the following characteristics:

1. Allows the simultaneous treatment of all disturbances going to the plant and predicts the sets of disturbances that cause the worst case of constraint violation.
2. Can be applied either to linear or nonlinear systems.
3. Uncertainties in the model formulation (such as change in process parameter) can be included in a systematic way.

The open-loop backoff calculations were successfully applied to three illustrative examples.

Current work is under way to consider dynamic situations, both with and without controllers. This will lead us to the dynamic open-loop and closed-loop backoff problem. Also, we are currently extending these ideas to include structural aspects in the problem formulation. In this way, the best design and control configurations, the best design parameters, and the best operating conditions (including controller parameters) could be selected (Bahri et al., 1994).

Notation

C^1, C^2 = concentrations in the first and second CSTR
C_F = feed concentration
$\text{Cool}^1, \text{Cool}^2$ = amount of cooling in the first and second CSTR
F = set of feasible regions
g = set of inequality constraints
$G(s)$ = linear transfer function of system
$G_d(s)$ = disturbance transfer function
h = set of equality constraints
M_E = number of equality constraints
M_I = number of inequality constraints
$\boldsymbol{p}_p$ = vector of process parameters
Q_F^1, Q_F^2 = first and second feed flow rates
T^1, T^2 = temperatures in the first and second CSTR
T_F = feed temperature
$\boldsymbol{u}(s)$ = vector of inputs to the linear system
$\boldsymbol{x}$ = vector of inputs to the linear system
$y(s)$ = vector of outputs from the linear system
z = vector of optimization variables
z^0, z_L, z_U = optimal value, lower, and upper bounds for optimization variables
z^+, z^- = positive and negative corrections to x^0
Φ = objective function

Greek letters

$\boldsymbol{\theta}$ = vector of disturbances
$\theta^N, \theta^L, \theta^U$ = nominal values, lower and upper bounds for disturbances
Φ = objective function
Γ = set of all possible realizations of disturbances

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