Integrated Flexibility and Controllability Analysis in Design of Chemical Processes

Parisa A. Bahri, Jose A. Bandoni, and Jose A. Romagnoli
ICI Laboratory of Process Systems Engineering, Dept. of Chemical Engineering,
The University of Sydney, Sydney, NSW 2006, Australia

A systematic approach for the synthesis of flexible and controllable plants is presented. It provides a new quantitative measure of the flexibility and controllability of a design and allows the designer to systematically evaluate different process structures and/or control systems. An integrated approach based on the dynamic mixed-integer nonlinear-programming problem is introduced that consists of two stages in each iteration of the algorithm. In this way, the effect of disturbances on the process design and operation, as well as its ideal performance, under a variety of control schemes can be estimated. The method is illustrated using a mini-integrated plant as a case study.

Introduction

Increased process integration and tight operating conditions are putting greater demands on plant control-system performance than at any time in the past. If a plant is designed only on the basis of steady-state economic considerations, then it is not uncommon that unfavorable process dynamics make the design of a satisfactorily working control system impossible.

Thus, a good process design must not only exhibit an optimal balance between capital and operating costs, it must also exhibit operability characteristics that will allow economic performance to be realizable in a practical operating environment. From the control point of view, operability can be broken down into a set of plant properties, operating conditions, and decisions to be made during operability assessment (Wolff et al., 1994), such as stability of the plant, optimality, measurements, manipulated inputs, flexibility, and controllability (that depends on the type of controller implemented in the plant). To use the analysis tools outlined, Wolff et al. (1994) applied those issues in an order that was determined from relationships between them. Obviously all these aspects interact in a more complicated way than that implied by a sequential treatment.

It is the purpose of this article to present an integrated methodology for considering different issues in operability assessment, especially flexibility and controllability. A framework within an optimization environment is proposed that incorporates optimality (this includes the synthesis and design as well), flexibility, and controllability (including selection of controllers). An interative methodology has been used first by Bandoni et al. (1994) and Bahri et al. (1994, 1995, 1996) in order to analyze the steady-state flexibility of a chemical plant. In this method, to ensure the feasible operation of the plant, the optimum point is moved to somewhere inside the feasible region (called back-off point). Therefore having disturbances in the system will not cause any constraint violation. The amount of back-off can be used as a measure of the flexibility of the plant. The algorithm for calculation of back-off consists of two stages called outer and inner loops, and each loop has been formulated as a semi-infinite optimization problem. Outer loops give the best operating conditions for a given set of disturbances. In the inner loops, the feasibility of the operating conditions proposed in the last outer loop are tested. In this stage, the disturbance realizations that produce most constraint violations are found (if any) and passed to the next outer loop. The outer loop in each iteration of the steady-state open-loop back-off calculation can be formulated as follows (Bahri et al., 1996):

$$\min_{z} \Phi\left(z, x, \theta^N, p_p\right) \qquad \text{(P1)}$$

subject to

Correspondence concerning this article should be addressed to P. A Bahri.
J. A. Bandoni is also with PLAPIQUI (UNS-CONICET), 12 de Octubre 1842, (8000) Bahia Blanca, Argentina.

$$h_i(z, x, \theta^k, p_p) = 0 \qquad i \in E$$
$$g_j(z, x, \theta^k, p_p) \le 0 \qquad j \in I$$
$$z \in Z = \{z : z^L \le z \le z^U\}$$
$$\theta^k \in \Gamma,$$

where

z = vector of independent (decision) variables
x = vector of state variables
θ^N = nominal value of disturbances
θ^k = the combination of disturbances found in the previous inner loops
p_p = vector of process parameters
E, I = set of indexes of equality and inequality constraints, respectively

Γ is a region containing all the possible realizations of the disturbances, which is defined as

$$\Gamma = \{\theta : \theta^L \le \theta \le \theta^U\}. \qquad (1)$$

As discussed in the previously cited references, since a uniform distribution for disturbances is assumed, any choice of $\theta \in \Gamma$ is considered to be equally probable. Each different combination of disturbances generates a different feasible region that is characterized as

$$F^k = F(z, x, \theta^k, p_p) = \{z : h_i(z, x, \theta^k, p_p) = 0,$$
$$g_j(z, x, \theta^k, p_p) \le 0, \quad z \in Z, \quad i \in E, \quad j \in I\}. \qquad (2)$$

Assuming z^* to be the optimal vector corresponding to the outer loop in one of the iterations, for each of the inequality constraints, the realization of disturbances around the point z^*, which produces the most violation of that constraint, is found in the inner loop. Therefore, in the inner loop of each iteration, the following optimization can be formulated for each $j \in I$:

$$\max_{\theta} g_j(\theta, z^*, x, p_p) \qquad (P2)$$

subject to

$$h_i(\theta, z^*, x, p_p) = 0 \qquad i \in E$$
$$\theta \in \Gamma.$$

If no constraint is violated in this step, the algorithm stops, otherwise, the vector(s) found from the solution of problem P2 is passed to the outer loop of the next iteration. After the algorithm converges, the final feasible region, which is the intersection of all the feasible regions corresponding to different disturbance combinations found in different inner loops, is referred to as the permanent feasible region (PFR), which is the region in which the plant will always operate feasibly, even in the presence of disturbances. The permanent feasible point (i.e., the back-off point) belongs to the PFR and comes from the last outer loop solution.

Later, Figueroa et al. (1996) incorporated the dynamics of the plant into the flexibility analysis, and also considered the effect of different controllers on the controllability of a process without any intention for retrofit design.

In this article, the procedure developed for steady-state flexibility is modified in order to consider the dynamic situation as well as the possibility of structural changes (both in design and control). As a result, the following will be achieved:

1. Steady-state and dynamic flexibility analysis in process design
2. Flexibility and controllability analysis of process design.

As the starting point, the superstructure of a flow-sheet example will be developed. After this, in order to avoid a very complex problem that is hard to solve, the measurements and manipulated variables of the system are considered to be known. The next step is the optimality, flexibility, and controllability analysis of this plant, all of which are embedded within the proposed algorithm. This results in dynamic mixed-integer nonlinear-programming (MINLP) and/or nonlinear-programming (NLP) problems that can be solved by the use of existing techniques. Therefore, this interesting example can be used to evaluate the applicability of this methodology. Furthermore, this study can provide some insights into the effect of using model-based controllers (in this case a DICOF controller) in the flexibility and controllability of a design. Therefore, the model can also be used as a tool in making the comparison between conventional and advanced controllers.

Optimal Process Synthesis, Design, and Operation with Uncertainty

Over the past two decades, increasing attention has been paid to the problem of systematically incorporating flexibility in the synthesis and design of chemical processes. Some other works have concentrated on the problem of redesigning an existing process to increase its flexibility (Pistikopoulos and Grossmann, 1988). However, there are few works that analyze both the flexibility and controllability of a plant. In this work we first look at the problem of improving the flexibility of a plant through its retrofit design, after which we look at the controllability aspects as well.

Flexibility considerations in chemical process design

Flexibility is one of the most important issues in analyzing the operability of chemical plants, since it gives a measure of the capability of a process to operate feasibly over a range of disturbances. Bahri et al. (1996) give a brief review of earlier works in this area, and also make a comparison between some of those methods and their proposed procedure.

In order to incorporate the flexibility problem in design and synthesis, one can use the methodology described in the preceding section, to find the best flow sheet and design parameters or the best design changes possible, which results in a plant with the least back-off from the original economic optimum. For this case, there still exists two major steps in each iteration of the back-off calculation (outer and inner loops), but because of the structural considerations, the outer loop becomes an MINLP optimization problem, and the inner loops remain as NLP. Therefore, the flow sheet, design parameters, and other decision variables will be selected in the outer loop, and the feasibility of the selected system for the given range of disturbances will be tested in the inner loops. The outer loop of the *flexibility* problem together with design considerations can be formulated as follows:

$$\min_{z,d,y} \Phi\left(z, d, y, x, \theta^N, p_p\right) \tag{P3}$$

subject to:

$$h_i\left(z, d, y, x, \theta^k, p_p\right) = 0 \qquad i \in E$$

$$g_j\left(z, d, y, x, \theta^k, p_p\right) \le 0 \qquad j \in I$$

$$z \in Z = \{z : z^L \le z \le z^U\}$$

$$y \in \{0,1\}$$

$$\theta^k \in \Gamma,$$

where
y = vector of integer variables
d = vector of design variables

In this case, the vector θ^k comes from the previous inner loop, except for the first iteration, in which: $\theta^k = \theta^N$. In the same manner, the problem formulation for the inner loops of the steady-state open-loop back-off calculation of a process design is given as (for $j \in I$):

$$\max_{\theta} g_j(\theta, z^*, d^*, y^*, x, p_p) \tag{P4}$$

subject to

$$h_i(\theta, z^*, d^*, y^*, x, p_p) = 0 \qquad i \in E$$

$$\theta \in \Gamma,$$

where z^*, d^*, and y^* are the optimal solutions found in the outer loop. As with the inner level subproblems in the steady-state back-off calculation, if at this stage no constraint is violated (meaning that for all $j \in I$, $\max g_j \le 0$), the algorithm stops; otherwise, the combination(s) of disturbances that gives the most violation of constraint(s) (the optimal solution of the inner loops) will be passed to the outer loop of the next iteration.

As indicated by Grossmann (1989), in order to formulate the synthesis problem or any problem related to it, such as structural changes (e.g., problem P3), a representation containing all the alternative designs of flow sheets that are to be considered as an optimal solution, should be developed. This representation, known as superstructure, is of great importance, since the optimal solution can only be as good as the representation.

After a proper and systematic superstructure has been developed, the next step is to model the optimization problem. The synthesis and design problem consists of the selection of a flow sheet as well as design parameters. The former corresponds to discrete optimization, while the latter mostly belongs to continuous space. In this way, the synthesis problem results in an MINLP problem. In these kinds of problems, the modeling of discrete decisions is usually performed with 0-1 integer variables (variables y in problem P3). These variables can be assigned to each potential unit and/or stream.

There are several algorithms available for solving MINLP problems, which include:

1. Branch and bound
2. Generalized benders decomposition (GBD)
3. Outer approximation/equality relaxation (OA/ER)
4. Feasibility technique.

Viswanathan and Grossmann (1990) recently developed a new variant of the OA/ER algorithm that uses an augmented penalty function in the master problem (AP/OA/ER algorithm). This algorithm starts by solving a relaxed NLP problem, and at this stage, if an integer solution is found, the algorithm stops. Otherwise a mixed integer linear programming (MILP) master problem will be formulated. The procedure continues in an iterative manner until there is a decrease in the NLP solution. This algorithm has been implemented in the GAMS package (Brooke et al., 1992), which is used in this work. For more information on mixed-integer programming, the reader should see Floudas (1995).

Flexibility and controllability considerations in chemical process design

Interest in the interaction between process design and control has intensified in recent years, which has resulted in a significant increase in the amount of literature dedicated to this topic (Morari and Perkins, 1995; Luyben and Floudas, 1994a,b). Until relatively recently most controllability assessment has been concerned with the attainability of perfect plant control, limited by the factors that prevent physically realizable inversions of the plant transfer function. The two approaches along these lines are: (1) dynamic resiliency as proposed by Palazoglu and Arkun (1987), and (2) functional controllability as proposed by Perkins and Wong (1985). Recently, as an alternative to controllability assessment studies, Narraway and Perkins (1994) considered the selection of economically optimal regulatory control structures from the set of all possible measurements and manipulated variables using MINLP programming. In this work, they tried to incorporate the flexibility analysis (feasibility of the operation for a plant with a fixed design), assuming one disturbance to perturb the system. Consideration of both the flexibility and controllability aspects in synthesis and design of a process results in a plant that is not only flexible but also exhibits good dynamic performance. In other words, flexibility is not only an inherent quality of the chosen design and the operating point but also depends on the selected controller type and control structure. Therefore, considering the presence of controller(s) or even the possibility of choosing between different control structures or types of controllers during the flexibility study in design and operation, may result in a quite different structure and design. To do this, one might start with the procedure discussed in previous sections for steady-state back-off calculation to study the flexibility of a process design. Then, having determined the economic penalty associated with this back-off, one can estimate the potential recovery that various control schemes or control structures might provide. This gives a measure of the controllability together with the flexibility of the plant. In this step, the structure selected in the steady-state case may or may not be changed. Obviously, this depends on the type of controller used or the control structure selected in the plant. It should be seen that, for open-loop back-off calculation, a more realistic situation may be considered by allowing for the dynamic open-loop response of the process to the disturbances, again with or without design changes. In this case, what happens during the transient response of the system will be clear.

When calculating the dynamic open-loop and closed-loop back-off, the algebraic optimization problems given for the outer and inner loops (problems P1 and P2) become dynamic optimization problems, or in the case of design considerations, problem P3 changes into a dynamic MINLP problem. In a dynamic optimization or optimal control problem, besides the elements of an algebraic optimization problem, such as objective function and algebraic equality and inequality constraints, the set of differential equalities representing the dynamics of the system are incorporated as constraints. One way to solve this kind of problem is by embedding a differential equation solver into the optimization strategy. Then the optimization algorithm chooses the control profile or decision variables, and requires the integrator to solve the differential equations and find the values for objective function and constraints (sequential simulation and optimization). Recently other methods have been developed that avoid the need for simultaneously converging to the optimum while solving the differential equations. In this method, using some kind of polynomial approximation, such as orthogonal collocation on finite elements, the differential equations are converted to algebraic ones. The resulting algebraic equations are then written as part of an NLP problem that is solved within an optimization framework (Biegler, 1984; Biegler and Cuthrell, 1987, 1989; Logsdon and Biegler, 1989). The first approach can be computationally very expensive, even for small problems, as it tends to converge slowly and requires the solution of a set of differential equations at each iteration; however the numerical error of integration is normally small. The second approach does not require the solution of differential equations at each iteration; instead, it solves a simultaneous optimization and collocation problem, which is a faster method. This approach is very powerful, since it uses a fully algebraic formulation where it is easy to accommodate bounds for the manipulated variables, and it can be solved with any standard optimization solver. The main drawbacks are that discretizing the differential equations makes the problem's dimensions very large plus the solution may not be as accurate as when integrators are used. Both of these drawbacks definitely depend on the case study. Usually in dealing with real applications, it is better to use an integrator since the size of the problem is big. Also in those cases where for some operational constraints the tolerance to error is very small, integration at each iteration of optimization gives more precise solutions. In the application presented in this article, since the GAMS package is used to solve the resulting MINLP problems in different stages of our algorithm, the discretization method is implemented in order to deal with dynamic optimization problems.

The formulations presented for steady-state back-off calculation in the preceding subsection can be extended to consider dynamic situations for both open-loop and closed-loop cases. Therefore, the problem formulation for outer loop (problem P3) becomes:

$$\min_{\bar{z},d,y} \Phi[\bar{z},d,y,m_{oz},p_{cz},x(t),m(t),w(t),\theta(t),p_p,p_{cp},m_{op},t]_{t=\hat{t}} \quad \text{(P5)}$$

subject to

$$h_i\left[\bar{z},d,y,m_{oz},p_{cz},x(t),w(t),m(t),\theta^k(t),p_p,p_{cp},m_{op},t\right]=0 \quad i\in E$$

$$g_j\left[\bar{z},d,y,m_{oz},p_{cz},x(t),w(t),m(t),\theta^k(t),p_p,p_{cp},m_{op},t\right]\le 0 \quad j\in I$$

$$\frac{dx(t)}{dt}=f\left(\bar{z},d,y,m_{oz},x(t),m(t),\theta^k(t),p_p,m_{op},t,t_f\right)$$

$$\frac{dw(t)}{dt}=f\left(m_{oz},p_{cz},x(t),w(t),m(t),\theta^k(t),p_p,p_{cp},m_{op},t,t_f\right)$$

$$\bar{z}\in\{z,u(t)\}$$

$$z\in Z=\{z:z^L\le z\le z^U\}$$

$$u(t)\in U=\{u:u^L\le u\le u^U\}$$

$$m_{oz}\in M=\{m_{oz}:m^L\le m_{oz}\le m^U\}$$

$$p_{cz}\in P=\{p_{cz}:p^L\le p_{cz}\le p^U\}$$

$$y\in\{0,1\}$$

$$\theta^k\in\Gamma$$

$$x(t=t_0)=x_0$$

$$w(t=t_0)=w_0$$

$$m(t=t_0)=m_{op} \quad \text{or} \quad m_{oz},$$

where

$m(t)$ = vector of manipulated variables
$w(t)$ = vector of state variables related to controller
t_0 = initial time
t_f = final time
$\hat{t}$ = the specific time in which the values of variables are used to calculate the objective function
p_c = vector of controller parameters $\in\{p_{cp},p_{cz}\}$
m_o = initial values for manipulated variables $\in\{m_{op},m_{oz}\}$

The subscript p is used for constant parameters and z for freed parameters. This formulation is given for the general case where the controllers are considered to be present in the plant, and in the case of dynamic open-loop back-off calculation, the equations and variables related to controllers can be easily removed. In this formulation it should be seen that the equality and inequality constraints, h_i and g_j, include both the plant model and the algebraic equations of the controller.

In problem (P5), the binary variables y are used for the selection of the best flow sheet and/or control structures. It should be mentioned that while the use of integer variables introduces a very important capability in the modeling of MINLP problems, inclusion of these variables also significantly increases the computational complexity of the optimization problem. The number of integer vectors that might yield a feasible solution to a bounded integer programming problem in n-dimensional space increases exponentially in n, and the computational effort has been shown by experiments to rise as the square of the number of integer variables for many types of the problems. Therefore, the way one models an MINLP problem can have a large impact on the performance of the MINLP algorithm. Another complication that may arise in these kinds of problems is when multiple steady states exist. By activating different binary variables, different steady states may be achieved. The proposed framework in this article does not consider this issue, making it something that needs further investigation.

As with outer loops, the formulation of the steady-state inner loops presented in the preceding subsection (problem P4) can be changed in order to consider the dynamic performance of the system, as follows:

$$\max_{\theta} g_j[\theta(t), \bar{z}^*, d^*, y^*, m_{oz}, p_{cz}^*, x(t), m(t), w(t), p_p, p_{cp}, m_{op}, t]_{t=t_{\max}} \quad \text{(P6)}$$

subject to

$$h_i(\theta(t), \bar{z}^*, d^*, y^*, m_{oz}^*, p_{cz}^*, x(t), w(t), m(t), p_p, p_{cp}, m_{op}, t) = 0 \quad i \in E$$

$$\frac{dx(t)}{dt} = f(\theta(t), \bar{z}^*, d^*, y^*, m_{oz}^*, x(t), m(t), p_p, m_{op}, t, t_f)$$

$$\frac{dw(t)}{dt} = f(\theta(t), m_{oz}^*, p_{cz}^*, x(t), w(t), m(t), p_p, p_{cp}, m_{op}, t, t_f)$$

$$\theta(t) \in \Gamma$$

$$x(t = t_0) = x_0$$

$$w(t = t_0) = w_0$$

$$m(t = t_0) = m_{op} \quad \text{or} \quad m_{oz}^*,$$

where

$t_{\max}$ = the time at which the amount of the constraint g_j is maximum

$\bar{z}^*, d^*, y^*, m_{oz}^*, p_{cz}^*$ = optimal solutions found in the outer loop

Figures 1a and 1b are diagrams of outer and inner loops of the closed-loop back-off calculation in the process design. In this figure, there is a box as an integrator that is used when the dynamic optimization problem is solved with sequential integration and optimization methods. In the case of dynamic open-loop back-off calculation in process design, the same diagrams can be used by removing the variables related to controllers; the integrator box should be eliminated from this diagram for the case of steady-state open-loop back-off calculation in process design.

Convergence considerations

As discussed in Bahri et al. (1996), global solutions for outer and inner loops are needed to guarantee the convergence of the back-off algorithm to a permanent feasible solution. For NLP cases, practical techniques such as *multistart techniques* can be applied to get global convergence. In the case of back-off calculations together with design considerations (steady-state or dynamic), the problem in outer loop becomes one of MINLP (problem P3 or P5). All the algorithms available for solving an MINLP problem need some form of convexity conditions in the functions of MINLP to be satisfied (Grossmann, 1989). For example, in the AP/OA/ER algorithm, if the convexity conditions are satisfied, the MILP master problem gives the lower bounds and the algorithm reduces to the OA/ER algorithm, except that it uses the solution of relaxed NLP as a starting point. This method shows a high degree of robustness with nonconvex problems.

As stated in the preceding subsection, the existence of multiple steady-state points also affects the convergence of the algorithm for both the steady-state and dynamic cases.

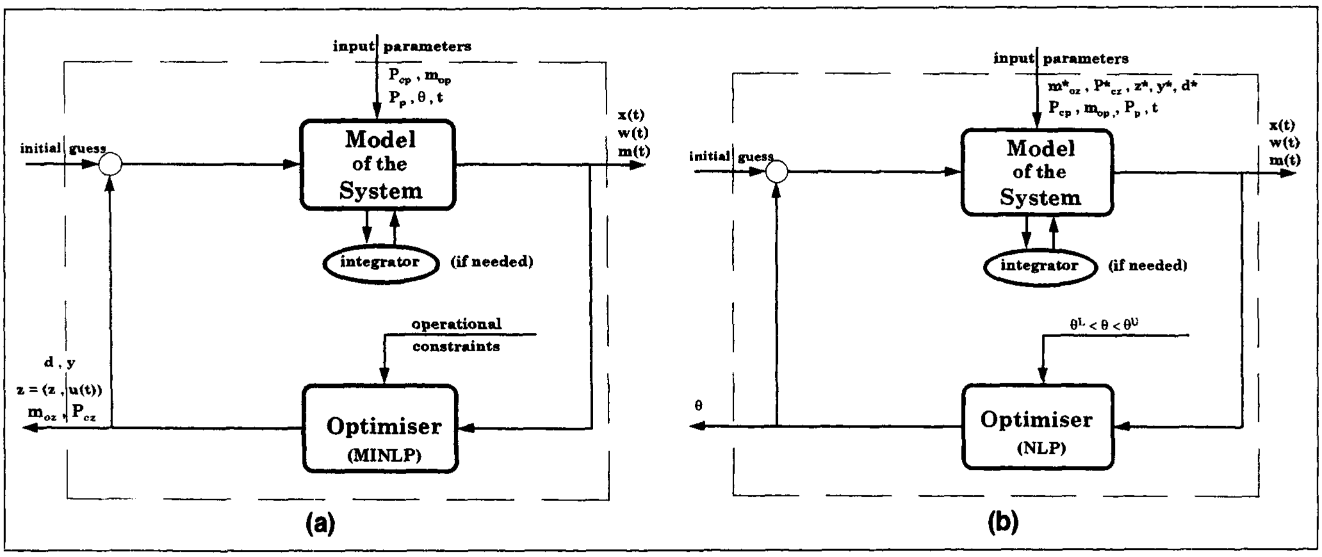

Figure 1. (a) Outer and (b) inner levels in the dynamic structural back-off calculation algorithm.

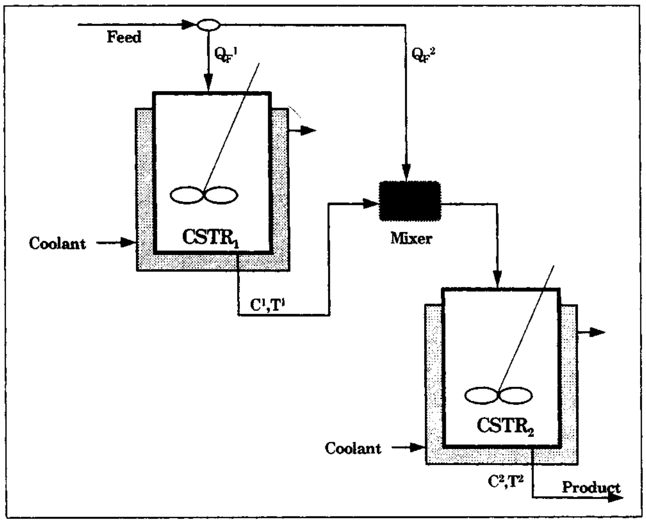

Figure 2. Flowsheet example: two CSTRs + mixer.

Illustrative Example

In this section, a flow-sheet example is considered to illustrate the application of the proposed algorithm. This relatively simple example will be used to illustrate the detailed steps of the back-off algorithm and its potential to be used in different areas (flexibility, controllability, etc.).

The flow sheet considered here (de Hennin and Perkins, 1991), consists of two continuous stirred-tank reactors (CSTR) with an intermediate mixer introducing the second feed (Figure 2). An exothermic irreversible first-order reaction $A \rightarrow B$ takes place in both reactors. The model equations are the material and energy balances around both the reactor and the mixer, and the inequality constraints used for optimization of the plant are as follows:

$$C1:\ T^1 \le 350, \qquad C2:\ T^2 \le 350$$
$$C3:\ Q_F^1 + Q_F^2 \le 0.8, \qquad C4:\ \text{Cool}^1 \le 30$$
$$C5:\ \text{Cool}^2 \le 20, \qquad C6:\ Q_F^1 \ge 0.05$$
$$C7:\ Q_F^2 \ge 0.05, \qquad C8:\ C^2 \le 0.3,$$

where

Cool^1 and Cool^2 = the amount of heat removed by coolants in the first and second CSTRs
T^1 and T^2 = the temperatures of the output streams from the first and second CSTRs
C^2 = the composition of the output stream from the second CSTR (product stream)
Q_F^1 and Q_F^2 = first and second feed flow rates

The objective function used for the optimization of this plant is the net profit of the operation, and the decision variables are considered to be the feed flow rates to the first CSTR and the mixer.

The possible disturbances entering the plant are considered to be both the feed temperatures and composition, for which the range of variation (lower bound, nominal values, and upper bounds) is given below:

$$T_F\ (\text{K}) = [298, 300, 315]$$
$$C_F\ (\text{mol/m}^3) = [19.5, 20, 21].$$

The optimization and back-off calculation for this plant have been done using package GAMS. The results from steady-state optimization with the nominal disturbance values are the optimum point at the intersection of constraints 1 and 5; the values for the objective function and the optimization variables are as follows:

$$\Phi = \$90.3522/\text{h}$$
$$Q_F^1 = 0.3552\ \text{m}^3/\text{s}$$
$$Q_F^2 = 0.2062\ \text{m}^3/\text{s}.$$

With the given disturbance bounds, the steady-state open-loop back-off point can be calculated using the procedure described before. The algorithm converges in three iterations, in which three of the constraints (C_1, C_5, and C_8) are violated due to the disturbance combinations given below (a summary of the progress of the algorithm is given in Bahri et al., 1996):

First combination: TF (K) = 315, CF (mol/m^3) = 21
Second combination: TF (K) = 298, CF (mol/m^3) = 19.5.

The result shows that for the open-loop case there is a back-off point that belongs to the PFR. At this point, the amount of the objective function and the number of decision variables are

$$\Phi = \$46.86/\text{h}$$
$$Q_F^1 = 0.252\ \text{m}^3/\text{s}$$
$$Q_F^2 = 0.055\ \text{m}^3/\text{s}.$$

Figures 3 and 4 show the nominal operating window and the PFR for this plant, together with the position of optimum and steady-state open-loop back-off points. As can be seen, there is about a 48% reduction in the amount of objective

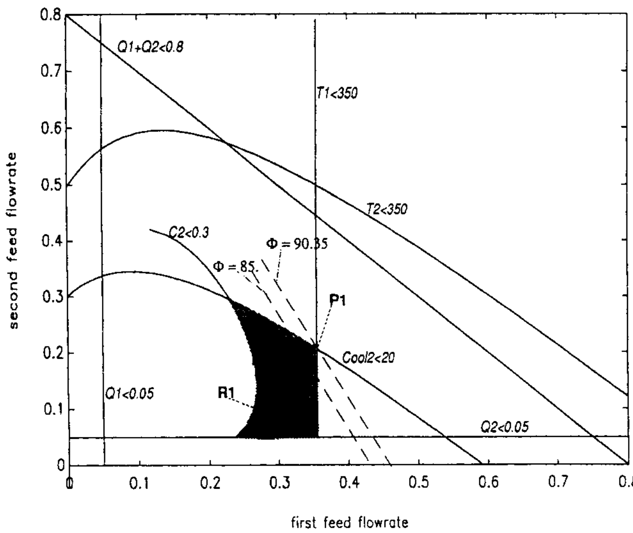

Figure 3. Nominal feasible region for two CSTRs.

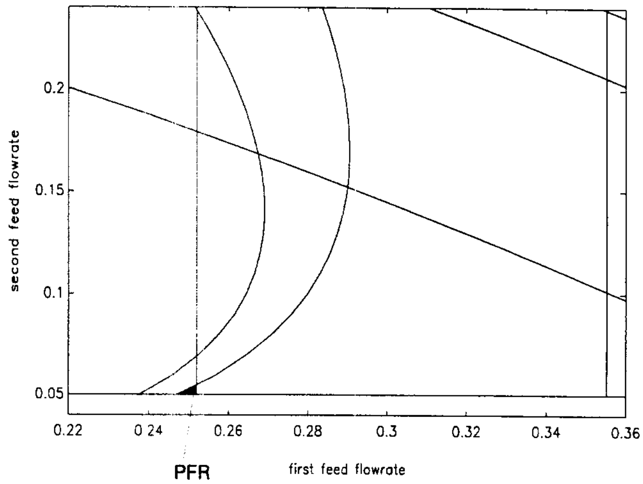

Figure 4. Permanent feasible region for two CSTRs.

function at the back-off point compared to the optimum one, which means that there is a large incentive to use some kind of control system and also to make some design changes in this plant, in order to recover some of the penalty due to open-loop back-off.

The results and discussion already given are taken from Bahri et al. (1996). In the present study, as a continuation of Bahri et al.'s work, several steps have been considered:

1. Dynamic open-loop back-off calculation for the original flow sheet
2. Closed-loop back-off calculation (using two different controllers—conventional and model-based—one at a time) for the original flow sheet
3. Steady-state open-loop back-off calculation in the retrofit design
4. Dynamic open-loop back-off calculation in the retrofit design
5. Closed-loop back-off calculation (using Ziegler-Nichols-tuned controllers in both CSTRs) in the retrofit design
6. Closed-loop back-off calculation (with both conventional and model-based options for the controllers) in the retrofit design.

In cases 2, 5 and 6, we assumed that the control structures in both reactors are fixed and considered to be (T^1, m^1) for the first CSTR and ($Cool^2$, m^2) for the second one. Variables m^1 and m^2 are the coolant flow rates in the first and second CSTR, respectively. In order to solve the resulting dynamic optimization problem for dynamic cases (open-loop and closed-loop) differential equations have been discretized using orthogonal collocation on the finite-element method.

Results

Figures 5 to 14 show the dynamic response of those system variables on which we have constraints to the two different disturbance combinations found during the steady-state open-loop back-off algorithm. In all these figures, the system is initially operating at the open-loop back-off point. From these figures, four facts can be concluded:

1. Figure 5 shows that by having the worst combination of disturbances in the system, the temperature of the first CSTR increases to the limit, but stays at that value. For the amount of cooling in the second CSTR, which is one of the active constraints at the optimum, its value remains below the limit even with disturbances (Figure 9).

2. Figures 6 and 7 show that despite the increase in the amount of cooling in the first CSTR and the temperature of the second one due to the disturbance combination of [315, 21], the constraints on these variables are never violated.

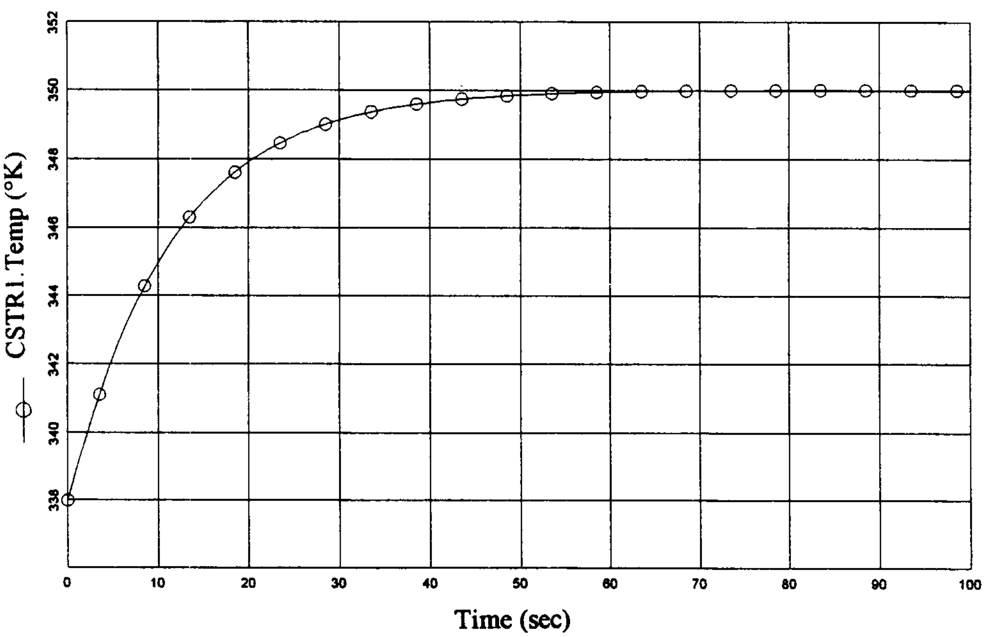

Figure 5. Dynamic response of the temperature in the first CSTR to the disturbance combination of $T_F = 315$, $C_F = 21$.
Starting from the steady-state open-loop back-off point.

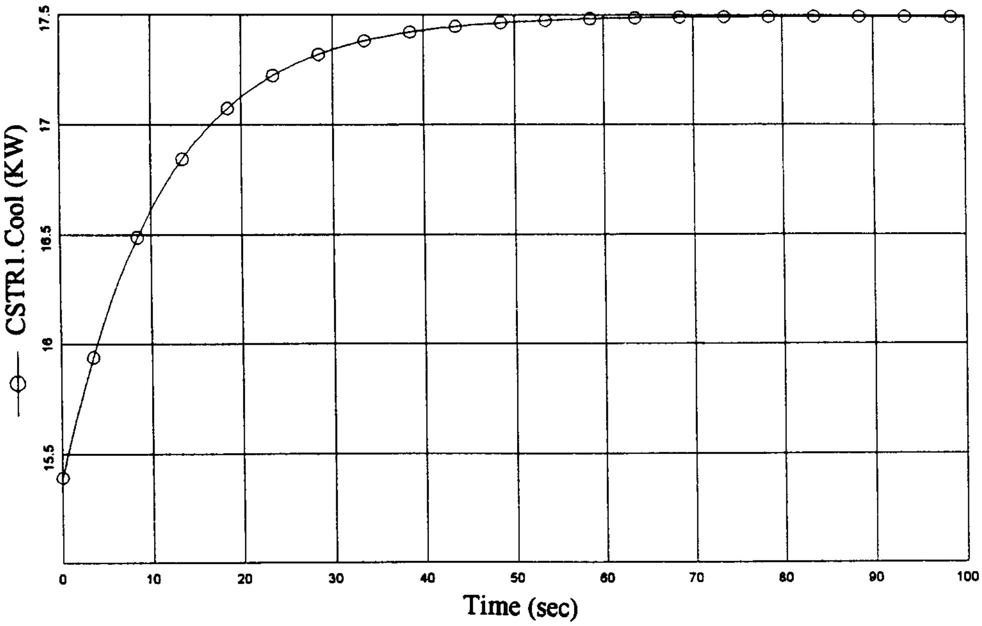

Figure 6. Dynamic response of the amount of cooling in the first CSTR to the disturbance combination of $T_F = 315$, $C_F = 21$.

Starting from the steady-state open-loop back-off point.

3. It can be seen in Figures 10, 11, 12 and 14 that with the disturbance combination as [298, 19.5], the temperatures and the amount of cooling in both CSTRs decrease, so there is no chance of constraint violation. But with this combination, the product composition increases (after an initial decrease), rising to 0.3 (Figure 13).

4. There is an inverse response in the product composition (C^2) in two different directions, depending on the realization of disturbances (Figures 8 and 13). For the combination of [315, 21], there is a peak in the response, and since we are looking at the initial and final steady-state conditions in the steady-state back-off calculation, this peak cannot be ob-

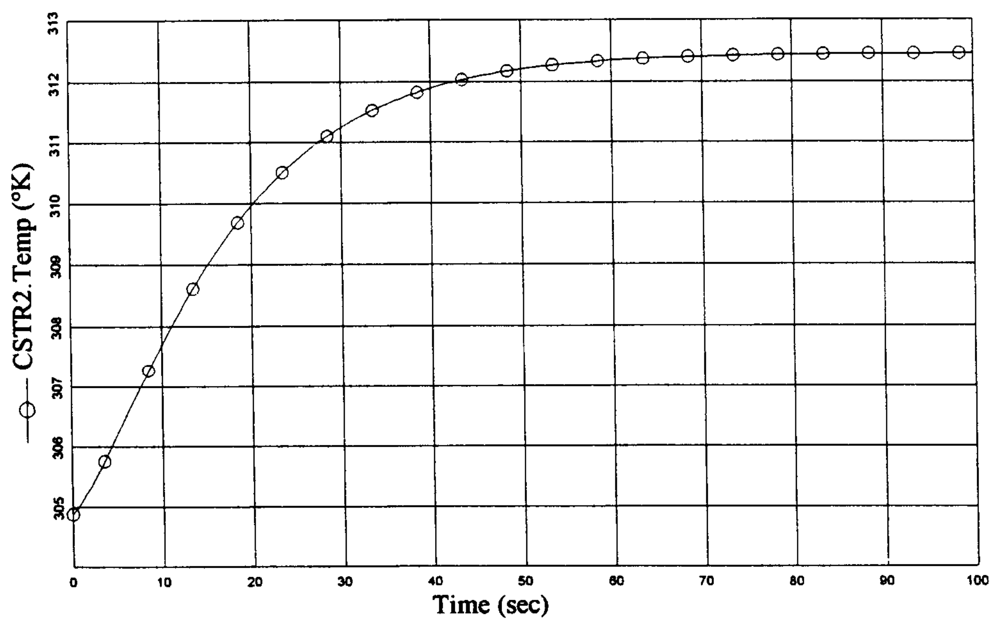

Figure 7. Dynamic response of the temperature in the second CSTR to the disturbance combination of $T_F = 315$, $C_F = 21$.

Starting from the steady-state open-loop back-off point.

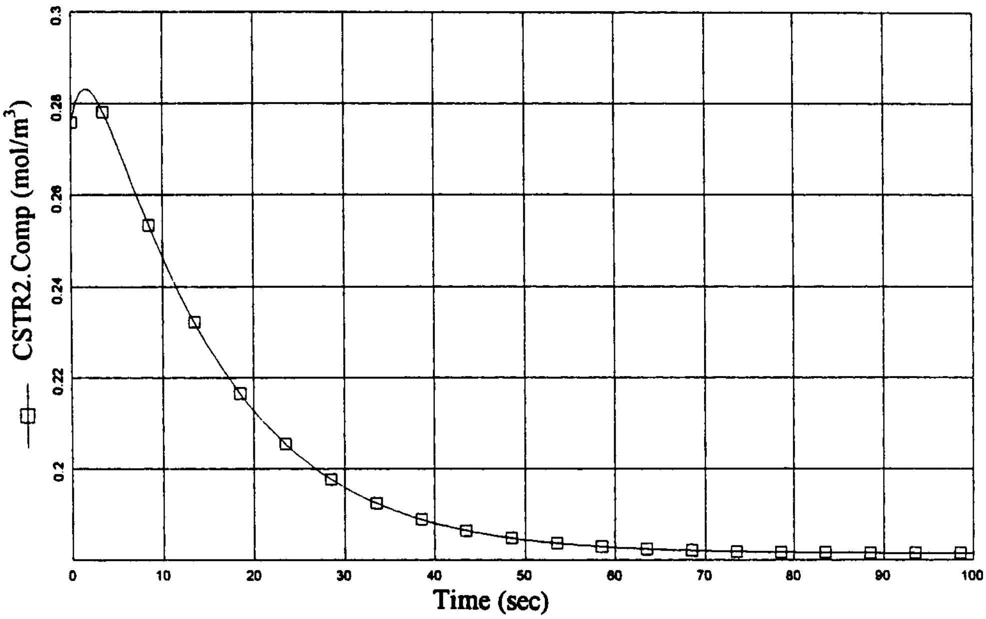

Figure 8. Dynamic response of the product composition in the second CSTR to the disturbance combination of $T_F = 315$, $C_F = 21$.

Starting from the steady-state open-loop back-off point.

served. Therefore, depending on the range of the disturbance variations, this peak may reach the limit or even violate the constraint. In that case, the results for steady-state and dynamic open-loop back-off will definitely be different. *Thus, for a plant with a given design, the flexibility analysis should be carried out in a dynamic environment.*

Because of the preceding results, we did the dynamic open-loop back-off calculation, as the first case in our work. The results for this and the other cases are given below.

Case 1. The results from the dynamic open-loop back-off calculation are exactly the same as for the steady-state calculation. This algorithm also converged in three iterations, and

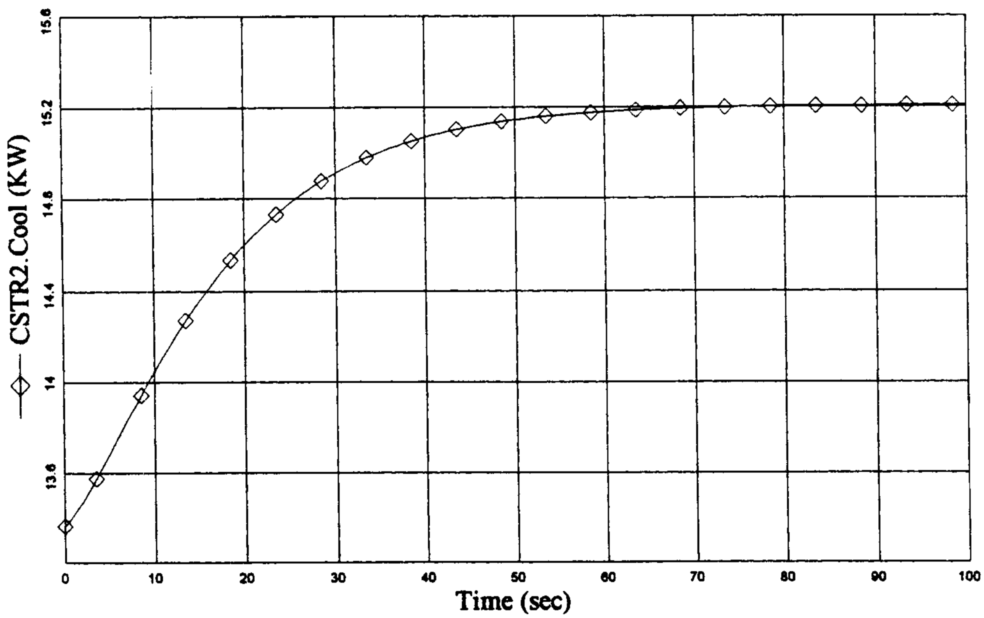

Figure 9. Dynamic response of the amount of cooling in the second CSTR to the disturbance combination of $T_F = 315$, $C_F = 21$.

Starting from the steady-state open-loop back-off point.

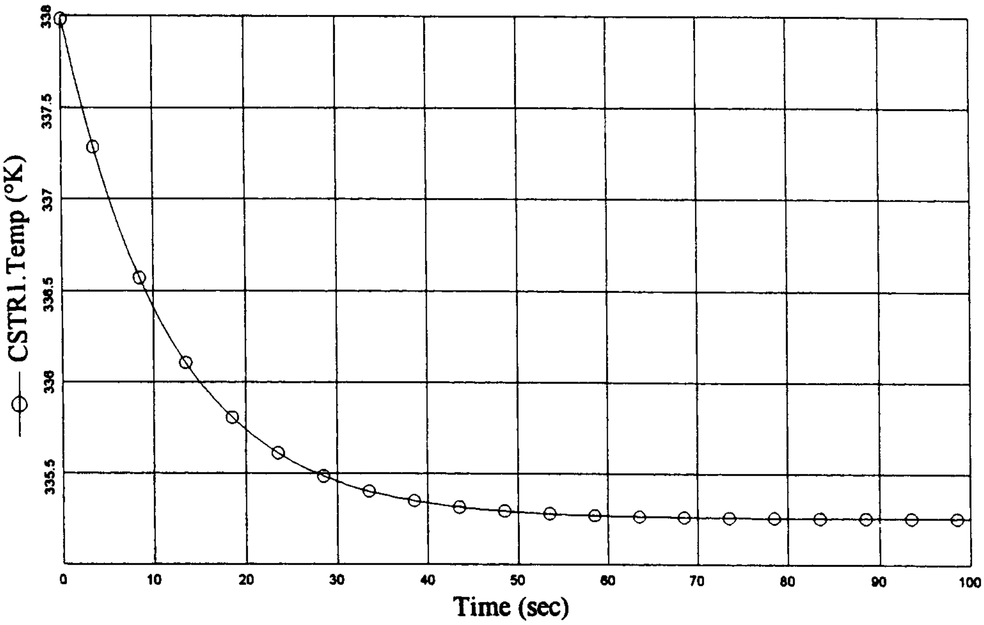

Figure 10. Dynamic response of the temperature in the first CSTR to the disturbance combination of $T_F = 298$, $C_F = 19.5$.

Starting from the steady-state open-loop back-off point.

the same disturbance combinations have been found in the inner loops. This result has also been verified with Figure 8. As can be seen, the peak on the response of the product composition is below the limit (0.3), which is why the steady-state and dynamic back-off points are the same.

Case 2. After the dynamic open-loop back-off calculation, the next step is to calculate how much of the loss due to open-loop back-off may be recovered, thus giving an idea of the controllability of the plant. In this case, using the control structures in both CSTRs as mentioned before, two different controllers were used (one at a time) to calculate the amount of closed-loop back-off necessary (the gains of the controllers

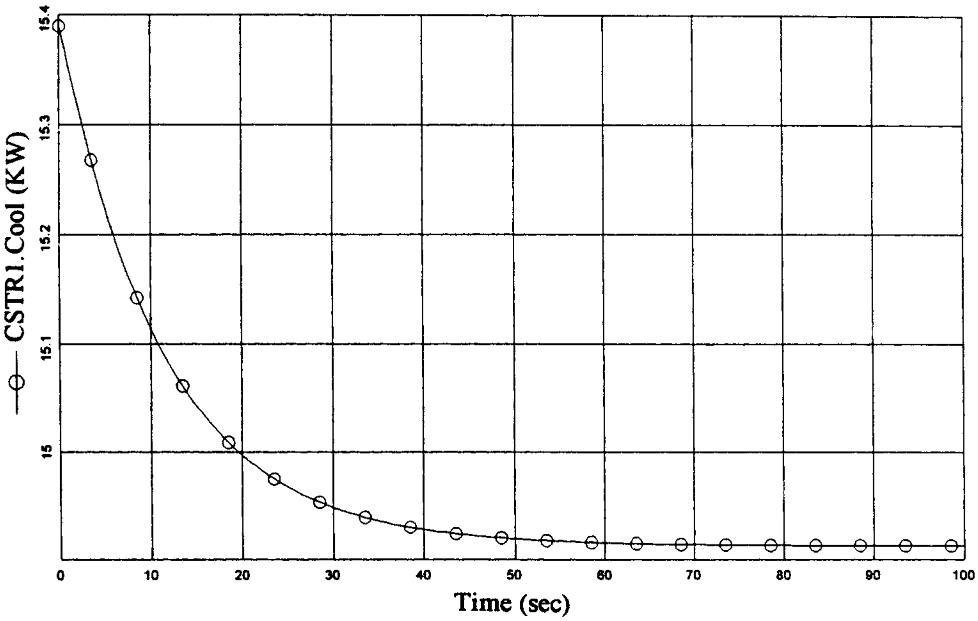

Figure 11. Dynamic response of the amount of cooling in the first CSTR to the disturbance combination of $T_F = 298$, $C_F = 19.5$.

Starting from the steady-state open-loop back-off point.

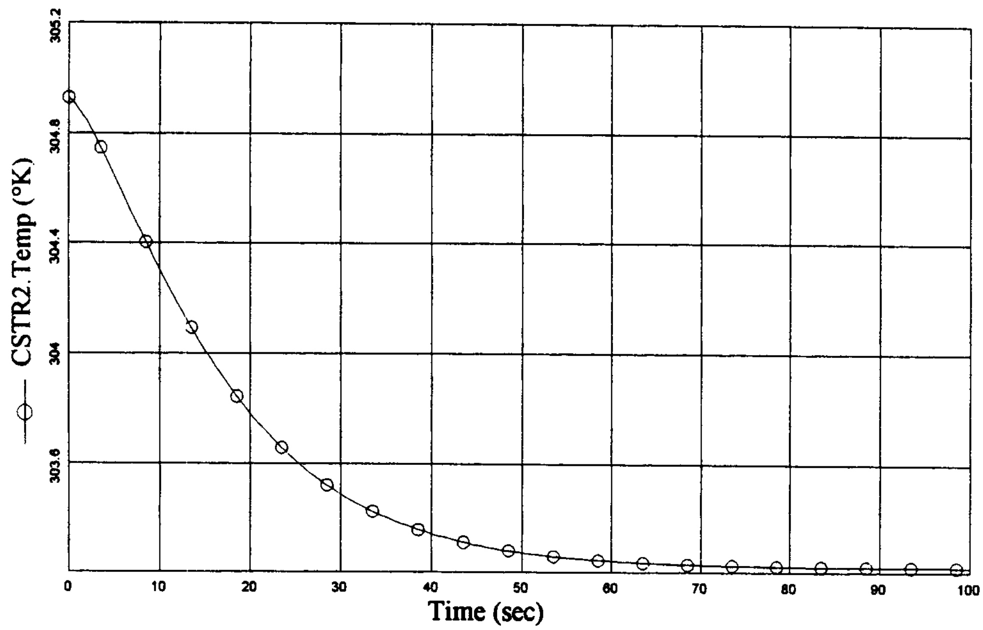

Figure 12. Dynamic response of the temperature in the second CSTR to the disturbance combination of $T_F = 298$, $C_F = 19.5$.

Starting from the steady-state open-loop back-off point.

are considered to be the additional decision variables). These controllers were:

1. A multiloop PI controller tuned by the Ziegler-Nichols method
2. A multivariable controller designed by package DICOF (Agamennoni and Romagnoli, 1993).

Table 1 shows the results from the open-loop and closed-loop back-off calculations. For this example, two things are quite clear. First, the difference in Φ between the nominal optimal conditions and the open-loop back-off case indicates that there is a significant economic incentive for some form of control scheme. Second, the use of a control scheme some-

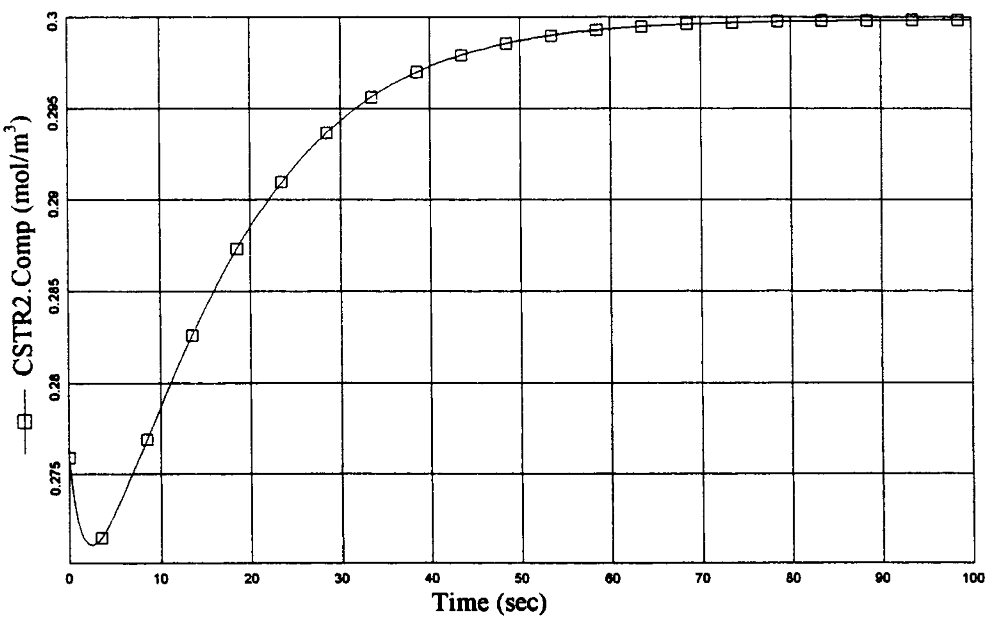

Figure 13. Dynamic response of the product composition in the second CSTR to the disturbance combination of $T_F = 298$, $C_F = 19.5$.

Starting from the steady-state open-loop back-off point.

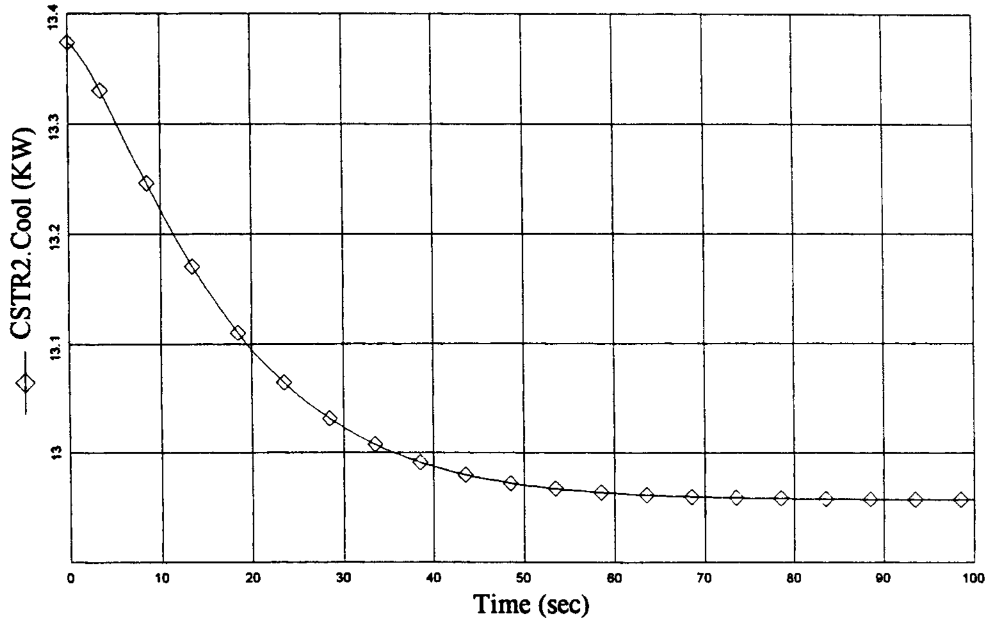

Figure 14. Dynamic response of the amount of cooling in the second CSTR to the disturbance combination of $T_F = 298$, $C_F = 19.5$.

Starting from the steady-state open-loop back-off point.

what more sophisticated than a Ziegler-Nichols-tuned multiloop controller (model-based) would seem to be economically warranted.

For the case of either Ziegler-Nichols or DICOF controllers, the back-off algorithm converges in two iterations with the disturbance combination found in the inner loop as [315, 21], and the other combination does not violate any of the constraints in the closed-loop system (especially the one on the product composition). This is because of the ability of the controllers to reject the effect of disturbances in both CSTRs. Therefore, less perturbations are transferred from the first reactor to the second one, and the product composition, C^2, will not be violated with the disturbance combination of [298, 19.5]. Figures 15 to 20 show the dynamic response of the temperature of the first CSTR (first controlled variable), the amount of cooling in the second CSTR (second controlled variable), and the product composition. In the latter case, the dynamic behavior of this variable has been checked in response to the disturbance combination [298, 19.5]. As can be seen, the final value of the composition is below the constraint value.

Using two different control schemes to compare the closed-loop behavior of the controlled variables of the system (T^1 and Cool^2) shows that the dynamic response of the system to the input perturbations using the DICOF controller is the best. One important fact about this controller is that it can be easily implemented as a standard controller.

Table 1. Amount of Objective Function and Decision Variables Found from Different Back-off Problems

	Q_F^1	Q_F^2	K_1^*	K_2^*	Φ
Nominal optimum	0.355	0.206	—	—	90.35
Steady-state open-loop back-off	0.252	0.055	—	—	46.86
Dynamic open-loop back-off	0.252	0.055	—	—	46.86
Closed-loop back-off (Z-N)	0.323	0.17	2.	0.5	78.24
Closed-loop back-off (DICOF)	0.354	0.195	2.	0.1	88.17

*K_1 and K_2 are two parameters multiplied by controllers gains.

Case 3. In this step, emphasis has shifted toward improving the operation and profitability of the existing plant by considering the possibility of redesigning it to optimally increase its flexibility in the face of disturbances. As mentioned in the subsection "Flexibility Considerations in Chemical Process Design," a superstructure containing all possible changes should be developed first. Figure 21 shows the superstructure considered for this plant. A mixer is added to the flow sheet after the second CSTR, and there is a possibility of having an extra stream coming out of the first CSTR to be mixed with the outlet from the second CSTR in this mixer. The volumes of both CSTRs can be changed: therefore, in the new formulation, they are considered as additional decision variables. The other optimization variables added to the problem are the flow rates of streams 3 and 4. Regarding this superstructure, four integer variables (y_1 to y_4) are designated between streams 1 and 4. Since one of streams (1 or 2) should exist, $y_1 + y_2 \geq 1$. In this step, the steady-state open-loop back-off calculation algorithm has been applied to this superstructure. The algorithm converged in three iterations, and the progress of the algorithm during the outer loop and inner loops of each iteration is summarized in Tables 2 and 3.

As the results in Table 2 show, the structure found in the first iteration did not change through the second iteration, with only the design parameters and operating conditions varying. In the inner loop of the second iteration, in addition to constraints $C1$ and $C5$, constraint $C8$ has been violated, but with a different combination of disturbances. Therefore,

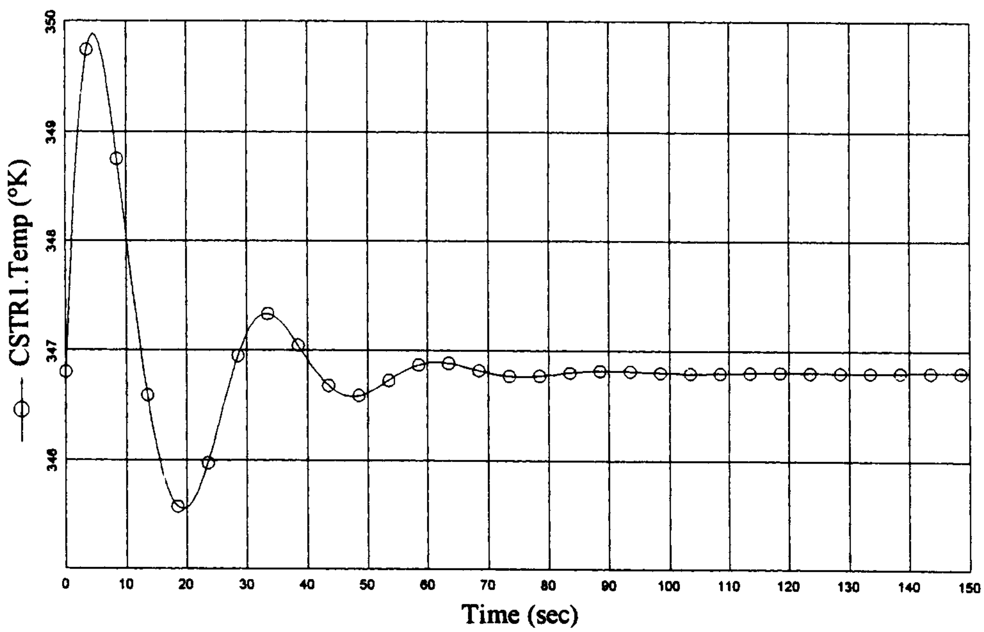

Figure 15. Dynamic response of the temperature in the first CSTR to the disturbance combination of $T_F = 315$, $C_F = 21$.
Starting from the Z-N closed-loop back-off point.

in order to deflect the effect of the disturbances as much as possible, a different structure has been chosen in the next outer loop. Otherwise, with the structure selected in the first and second iterations, despite having a larger nominal value for objective function, there would not be any permanent feasible point (back-off point) that would guarantee feasible operation of the plant in the face of the disturbance combinations found in the different inner loops. This shows the necessity of considering flexibility issues during the design stage. The structure chosen in the third iteration is the same as the structure given in Figure 21, and the permanent feasible region found is shown in Figure 22. It can be seen that the

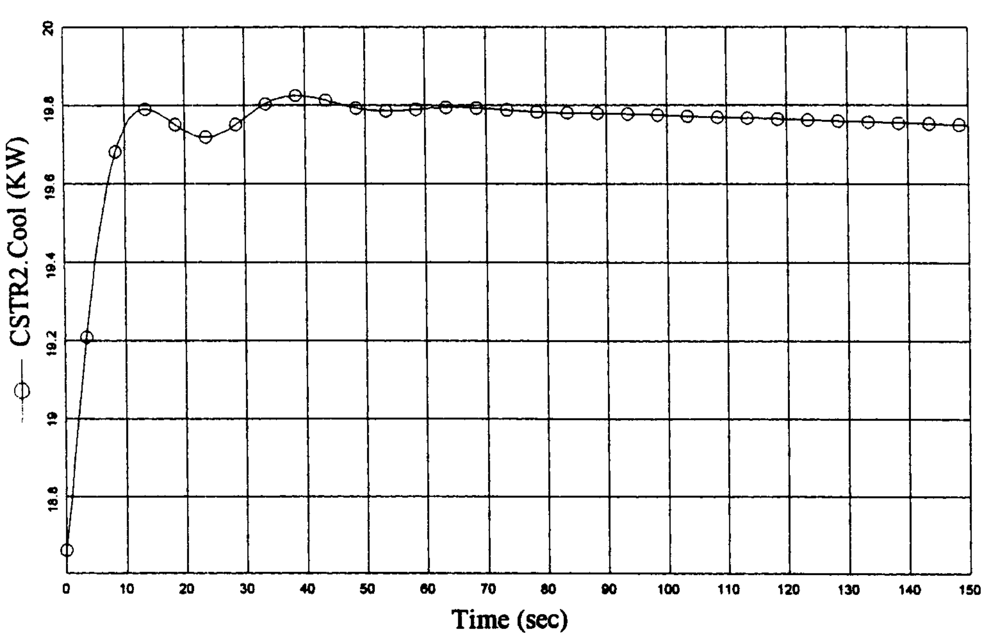

Figure 16. Dynamic response of the amount of cooling in the second CSTR to the disturbance combination of $T_F = 315$, $C_F = 21$.
Starting from the Z-N closed-loop back-off point.

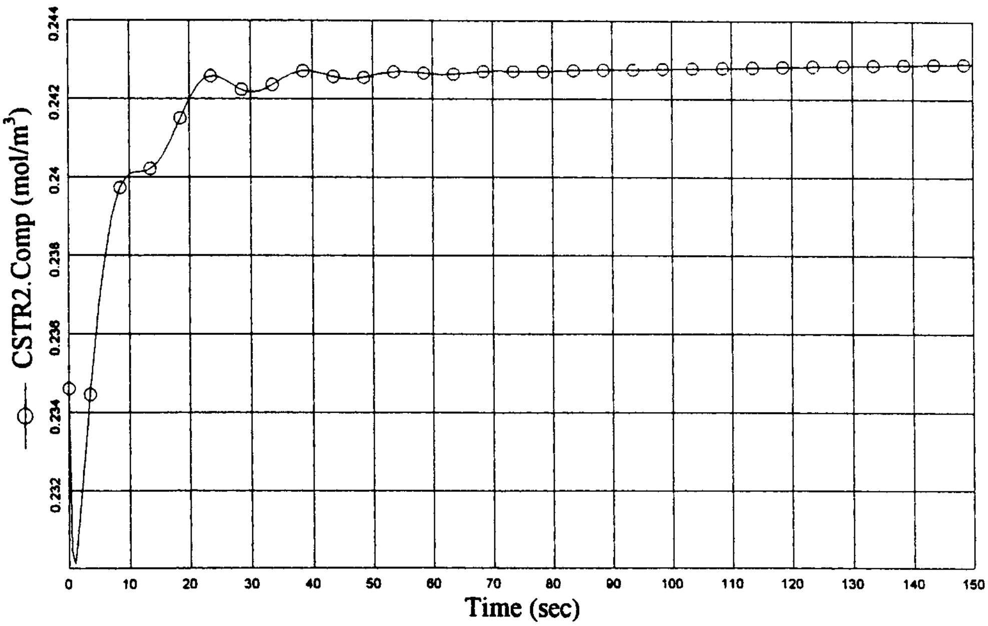

Figure 17. Dynamic response of the product composition in the second CSTR to the disturbance combination of $T_F = 298$, $C_F = 19.5$.

Starting from the Z-N closed-loop back-off point.

difference between Figures 22 and 4 comes from both the difference in structure and the volumes of reactors. In this case, the amount of objective function at back-off point is 58.6% greater than the one found in the steady-state open-loop case without design changes, which indicates the improvement achieved by the retrofit design of the plant.

Case 4. In this step, the dynamic effect of disturbances on the open-loop process has been considered. The problem status is exactly the same as in case 3, except for the presence of differential equations in the model of the system. Therefore, the subproblems in the outer and inner loops turn out to be dynamic optimization ones. Again, differential equations have

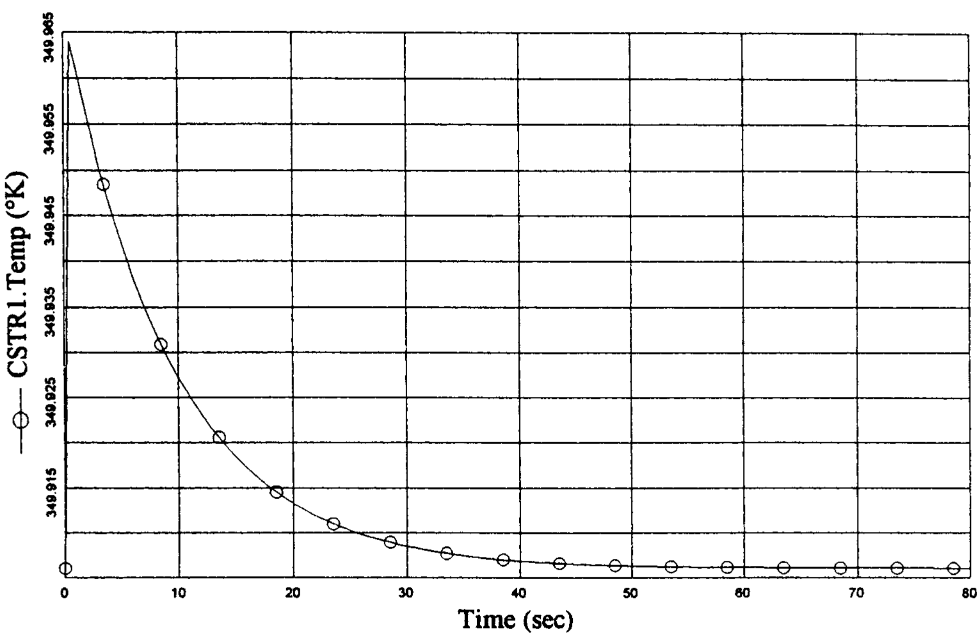

Figure 18. Dynamic response of temperature in the first CSTR to the disturbance combination of $T_F = 315$, $C_F = 21$.

Starting from the DICOF closed-loop back-off point.

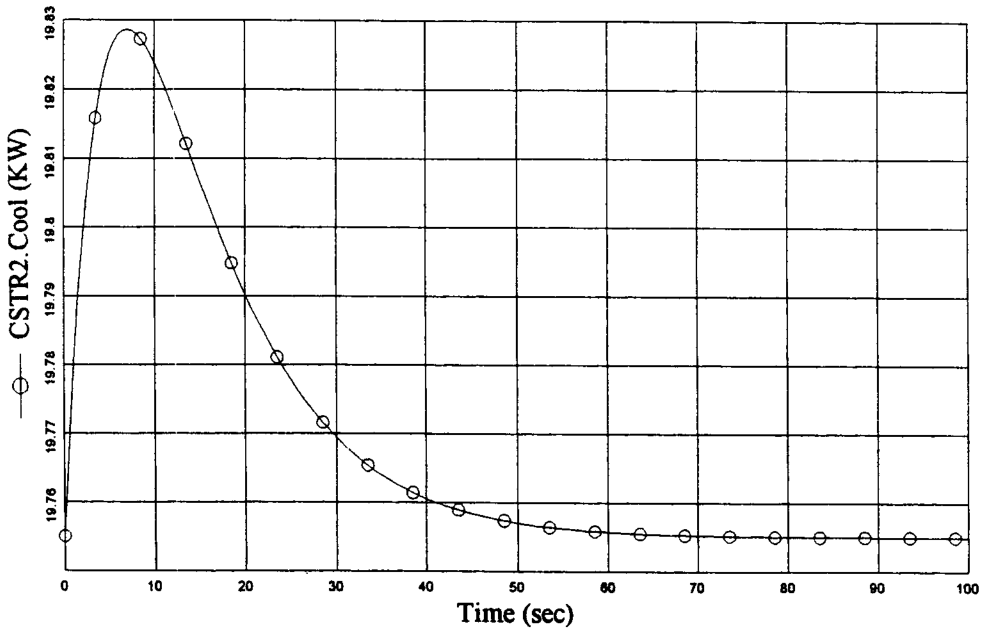

Figure 19. Dynamic response of the amount of cooling in the second CSTR to the disturbance combination of $T_F = 315$, $C_F = 21$.

Starting from the DICOF closed-loop back-off point.

been discretized using the simultaneous method, and taking the superstructure developed before into consideration, the structural dynamic open-loop back-off was calculated. Since the nominal values of the disturbances are considered in the first outer loop, the problem becomes a steady-state structural one, and the results are exactly the same as in case 3. In the inner loop of the first iteration, the problem is a dynamic one and the disturbance combination found is the one found in case 3. The second outer loop also gives the same feasible solution, despite the reverse behavior in the dynamic response of variable C^2 (product composition) to the disturbance combination found in the inner loop.

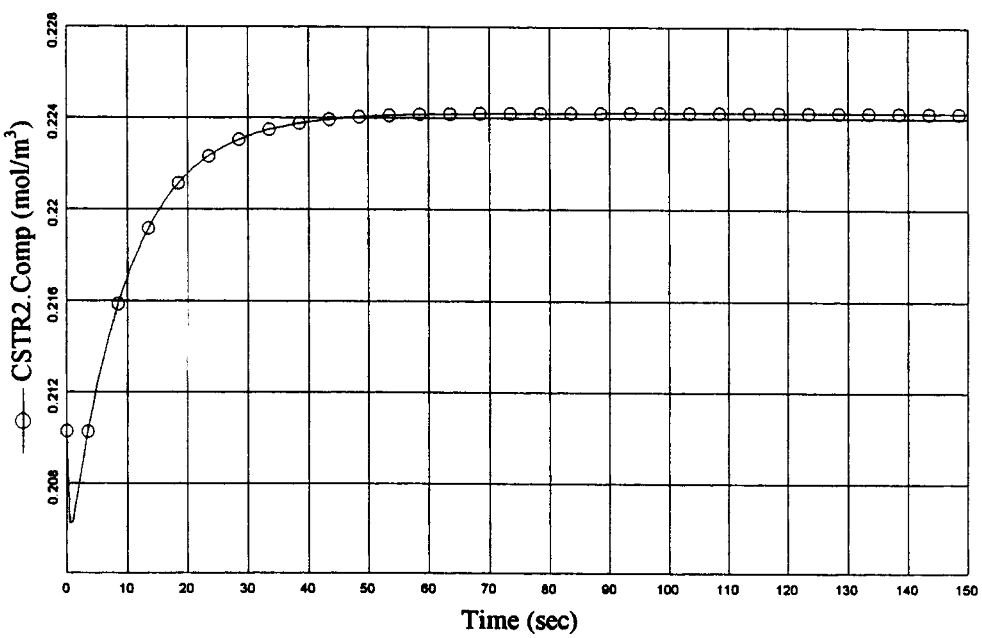

Figure 20. Dynamic response of the product composition in the second CSTR to the disturbance combination of $T_F = 298$, $C_F = 19.5$.

Starting from the DICOF closed-loop back-off point.

Table 2. Optimal Structure, Design Parameters, and Operating Conditions Found in the Outer Loop of Each Iteration of the Back-off Algorithm for Open-loop Case

Iteration	Q_1	Q_2	Q_3	Q_4	V_1	V_2	Φ
First	0.355	0.302	0.	0.355	4.5	4.5	108.74
Second	0.252	0.231	0.	0.252	4.5	5.03	76.90
Third	0.252	0.22	0.05	0.202	5.005	6.0	74.31

Table 3. Constraints Violated in the Inner Loops of Each Iteration of the Back-off Algorithm (Structural Open-Loop Case) and Relevant Disturbance Combinations

Iteration	Constraints Violated	Disturbances Combination (T_F, C_F)
First	$C1, C5$	(315, 21)
Second	$C1, C5-C8$	(315, 21)-(298, 19.5)
Third	None	Any

Case 5. The problem formulation in this case is exactly the same as in case 4, except for the presence of controller equations. The same superstructure has been considered in this section, and it is assumed that both CSTRs are controlled by conventional Ziegler-Nichols controllers. The control structures are considered to be the same as in case 2, which are (T^1, m^1) and (Cool^2, m^2) for the first and second CSTR, respectively. By applying the back-off algorithm to this problem, the best structure, together with the best design parameters, controller parameters, and operating conditions, can be calculated, thus achieving the most flexible and controllable plant with the least amount of closed-loop back-off. A summary of the progress of the algorithm through different outer and inner loops for this structural closed-loop back-off problem is given in Tables 4 and 5.

As can be seen, by using a multiloop conventional controller, say Ziegler-Nichols, there is a chance of choosing the best flow sheet for the nominal steady-state case (Figure 23), in order to improve the objective without endangering the flexibility of the plant. Therefore, through the back-off algorithm, the structure selected in the case of nominal disturbances (the first iteration) will not change, because the presence of controllers helps the plant to reject disturbances.

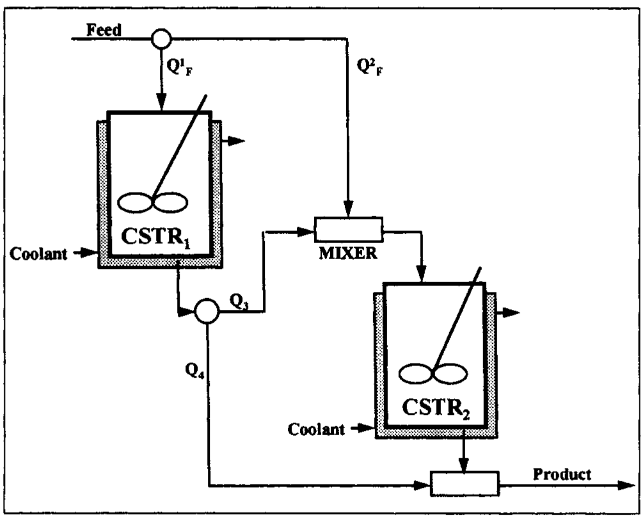

Figure 21. Superstructure for two CSTRs example.

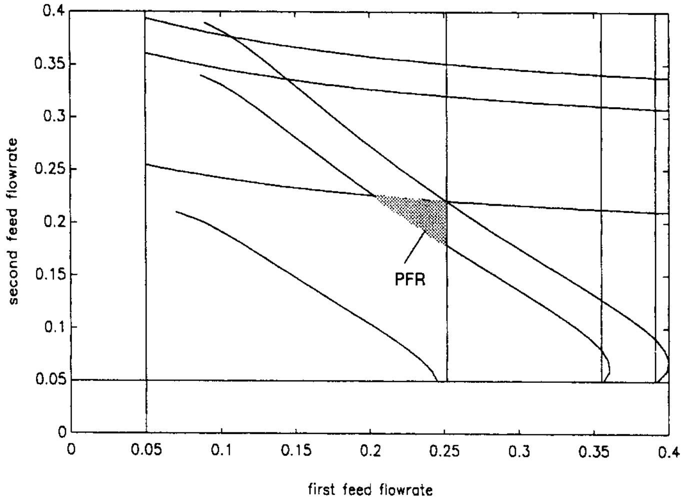

Figure 22. Permanent feasible region for the structure selected in steady-state structural back-off calculation.

Case 6. In this case, in addition to considering possible changes in design and flow-sheet structure, we assume that two types of controllers (the same as case 2) could be used for the CSTRs. Therefore, two other integer variables (y_5, y_6) are added to the problem. Also, as in the other closed-loop problems, the controller gains are among the decision variables. Again in this case, the first outer loop of the back-off algorithm is the steady-state structural one (because of the nominal values considered for disturbances), but since no information about the type of controller is transferred to the inner loop of the first iteration, the first inner loop problem will be an MINLP one, in order to find the most violations of the constraints along with the type of controller. In the first inner loop, the program gives the Z-N controller as the one that produces the bigger violation. In the second and third outer loops, the DICOF controller is seen to be the one that

Table 4. Optimal Structure, Design Parameters, and Operating Conditions Found in the Outer Loop of Each Iteration of the Back-off Algorithm for the Closed-loop Case with Z-N Controller

Iteration	Q_1	Q_2	Q_3	Q_4	V_1	V_2	K_1	K_2	Φ
First	0.355	0.302	0.	0.355	4.5	4.5	—	—	108.74
Second	0.316	0.245	0.	0.316	4.5	4.5	2.0	0.26	90.7

Table 5. Constraints Violated in the Inner Loops of Each Iteration of the Back-off Algorithm (Structural Closed-Loop Case with Z-N Controller) and Relevant Disturbance Combinations

Iteration	Constraints Violated	Disturbances Combination (T_F, C_F)
First	$C1, C5$	(315, 21)
Second	None	Any

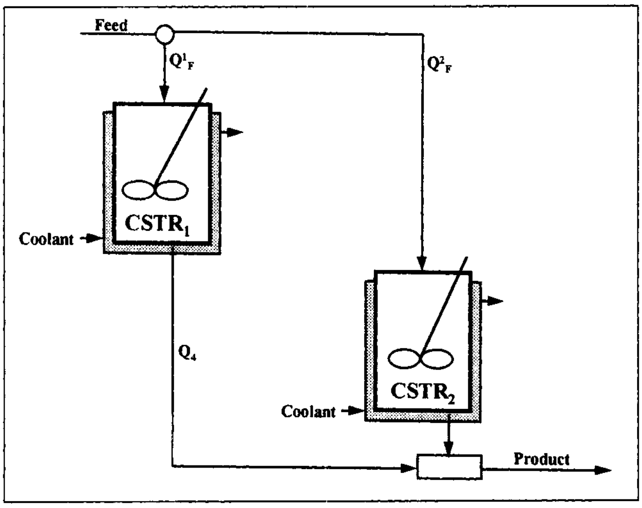

Figure 23. Structure selected by the nominal retrofit design or the structural closed-loop back-off calculations.

Table 6. Optimal Structure, Design Parameters, and Operating Conditions Found in the Outer Loop of Each Iteration of the Back-off Algorithm for Closed-Loop Case with DICOF Controller

Iteration	Q_1	Q_2	Q_3	Q_4	V_1	V_2	K_1	K_2	Φ
First	0.355	0.302	0.	0.355	4.5	4.5	—	—	108.74
Second	0.355	0.291	0.	0.355	4.5	4.5	2.0	0.1	106.83

Table 7. Constraints Violated in the Inner Loops of Each Iteration of the Back-off Algorithm (Structural Closed-Loop Case with DICOF Controller) and Relevant Disturbance Combinations

Iteration	Constraints Violated	Disturbances Combination (T_F, C_F)
First	$C1, C5$	(315, 21)
Second	None	Any

rejects the disturbances in both CSTRs better than the Z-N one does. A summary of the results found through the outer and inner loops of the back-off algorithm is given in Tables 6 and 7.

It can be seen from the results that, using the DICOF controller, we are able to reject disturbances as much as possible and therefore, there is a possibility of changing the structure to one that is more profitable. Comparing the results given in Tables 1 (for the DICOF case) and 6 shows that by changing the structure in Figure 2 to the one selected by the program in the present case (Figure 23), the profit of the plant can be increased by 27.2% by just relocating the mixer after the second CSTR and taking the second feed directly into the second reactor. The original volumes of both reactors were 5 m^3, and in the new structure they changed to 4.5 m^3 for the first CSTR and 6 m^3 for second one, respectively. Figures 24 to 26 show the dynamic response of the temperature of the first CSTR, the amount of cooling in the second CSTR, and the product composition in the new plant using the DICOF controller, to the disturbances, with the combination found by the back-off algorithm (Table 7).

Formulation of the optimization problems for the original flow sheet and also the proposed superstructure including one type of controller are given in the supplementary materials.

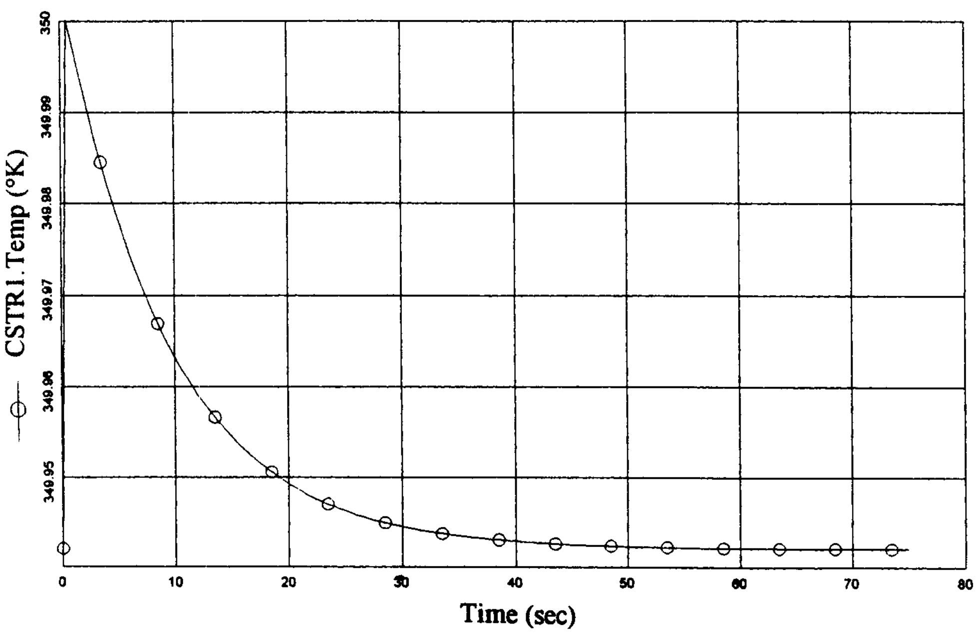

Figure 24. Dynamic response of temperature in the first CSTR to the disturbance combination of $T_F = 315$, $C_F = 21$.
Starting from the DICOF structural closed-loop back-off point.

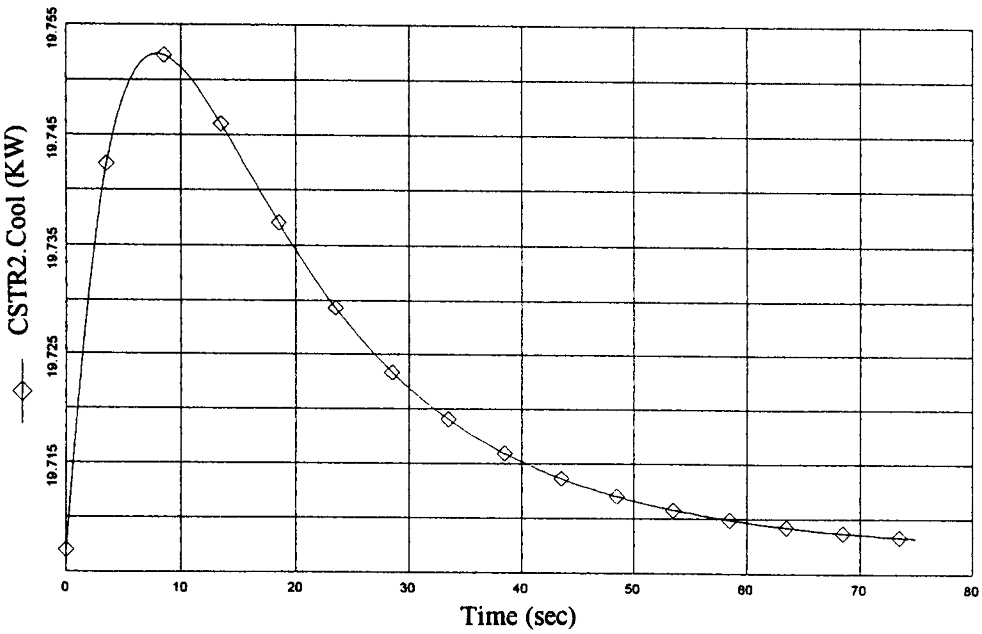

Figure 25. Dynamic response of the amount of cooling in the second CSTR to the disturbance combination of $T_F = 315$, $C_F = 21$.

Starting from the DICOF structural closed-loop back-off point.

Conclusion

In this article, the problem of interaction between design and control is addressed. A systematic approach was used in order to consider the controllability and flexibility aspects of a plant together with the possibility for retrofit design. This approach enables us to calculate the amount of back-off necessary from the nominal optimum of a plant to ensure the feasible operation of the plant in the face of disturbances. Using a flow-sheet example, first the effect of different controllers on the flexibility of a plant without considering any design changes was studied. The next step was to try to increase the plant's profitability by changing its structure and/or design parameters. It was found that by using some kind of model-based controllers (DICOF controller), one is able to switch to a structure that is more profitable without sacrificing the feasibility of the operation. In other words, *not only*

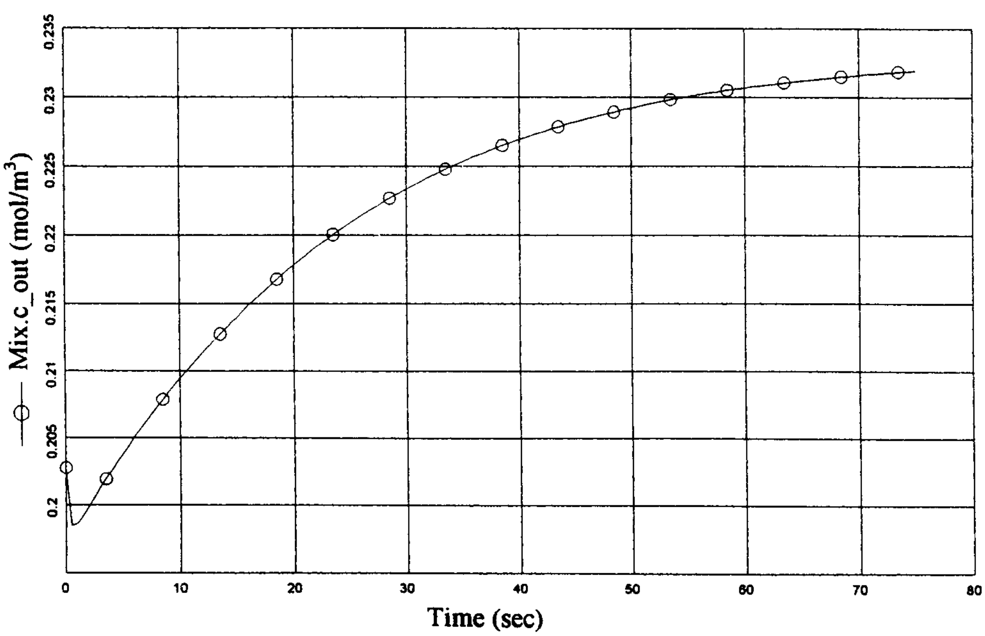

Figure 26. Dynamic response of the product composition to the disturbance combination of $T_F = 298$, $C_F = 19.5$.

Starting from the DICOF structural closed-loop back-off point.

the best performance that any controller can achieve on a plant is not only a function of the plant itself, but also the ability of a selected design to operate feasibly over a range of disturbances, depends on the type of controller.

Notation

F = set of feasible regions
g = set of inequality constraints
h = set of equality constraints
u = vector of control variables (time-dependent)
θ = vector of uncertain parameters
Φ = objective function

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