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Manuscript received June 3, 1983; revision received September 27, and accepted September 30, 1983.

Evaluation of Changeover Control Policies by Singular Value Analysis—Effects of Scaling

A method for assessing control performance at different operating conditions in a chemical process is developed using singular value analysis. The control potential of the system is established by analyzing the singular values of the steady-state system matrix. Dynamic considerations and interaction analysis can be included in the framework of the method described. The approach enables the process engineer to consider controllability of the process as well as economics in synthesizing a changeover control policy. Singular values depend on the scaling of the system, i.e., the definition of the physical dimensions of the system. The effects of scaling on the analysis are first investigated by scaling the steady-state system matrix with empirical methods, equilibration, and geometric scaling. Using the insights gained from these studies a scaling method, variable normalization and equation equilibration, which is intuitively appealing and suited for the purpose, is devised. Two typical chemical systems, continuous stirred tank reactor and a polymerization reaction system, demonstrate the usefulness of this method.

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SCOPE

The design of flexible chemical processes is an important problem facing a process systems engineer. The problem may be structured on three levels: (i) design of regulatory control structures, (ii) design of changeover control policies, and (iii) design of process structures. As one proceeds up the hierarchy, the flexibility of the system increases.

At the bottom level (i), the flexibility lies in the ability of the engineer to select various control interconnections to regulate the process. Several methods are described in the literature for selecting these interconnections (Bristol, 1966; Tung and Edgar, 1977; Witcher and McAvoy, 1977; Morari and Stephanopoulos, 1980; Romagnoli et al., 1980; Govind and Power, 1982; Gagnepain and Seborg, 1982; Lau et al., 1985; Jensen et al., 1982). However, the operating conditions and the process interconnections remain fixed.

At the intermediate level (ii), the operating conditions can be changed if better economic and control performance can be achieved. Consequently, both the control interconnections and the operating conditions can be altered. Algorithms also exist for selecting optimal conditions and for synthesizing the operating route to change from the current conditions to the new conditions (Arkun and Stephanopoulos, 1980; Prett and Gillette, 1980; Bamberger and Isermann, 1978; Garcia and Morari, 1981).

At the highest level (iii), the interconnections between process units become design variables in achieving the desired economic and operational goals. This lends a high degree of flexibility to the process. Morari and his coworkers (Lenhoff and Morari, 1982; Marselle et al., 1982; Morari, 1982, 1983; Morari et al., 1983) have studied this problem extensively, making significant advances toward the integration of process design, process operation, and process control.

In this paper we describe a method for evaluating the controllability of a process by singular value analysis. By plotting contours of the minimum singular value and the condition number of the steady-state system matrix over the feasible region, defined by the state and constraint equations, we can visualize the sensitivity and operability of the process system. This in turn provides a tool for designing changeover control policies. We also demonstrate how the concept of structural controllability of the system as defined by Morari and Stephanopoulos (1980) may be quantified through singular value analysis.

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Singular value analysis is a powerful tool for design of process control structures, one which is gaining widespread use. However, the scaling of the variables and equations affects the results of the analysis markedly. Therefore, for our approach to achieve reliable status in designing flexible chemical processes, this scaling problem must be resolved. Ideally, we would like a scale which permits us to analyze the intrinsic system behavior without confounding numerical artifacts. Our approach is to initially test well-known empirical methods, equilibration, and geometric scaling. Based on these studies we are able to devise a scaling method, variable normalization and equation equilibration, which is supported by physical considerations.

Finally, we demonstrate our approach by analyzing two typical systems: (1) a continuous stirred tank reactor with a first order endothermic reaction, and (2) a polymerization reactor. Particular emphasis is placed on the physical interpretation of the results.

CONCLUSIONS AND SIGNIFICANCE

A new method for analyzing changeover control policy for single chemical process units is developed using the singular value analysis of the steady-state system matrix. System control measures, sensitivity, and invertibility are evaluated over the processing unit's operating region defined by the state and constraint equations. Consequently, we can synthesize the control strategy based upon economic as well as controllability considerations. Extension to include dynamics and interaction of the system when designing the control policy can also be accomplished.

Singular value analysis depends on the scaling of the system, that is, the dimension of the physical variables. Unfortunately, no optimal scaling method exists for a general matrix defined on a vector space with an euclidean norm, although optimal scaling methods do exist for other norms (Bauer, 1963). Nevertheless, we have to ensure that the scale of the system does not obscure the real system behavior. Furthermore, our analysis shows that the appropriate indicator of the controllability of a system is not necessarily the absolute magnitude of the condition number (or minimum singular value), but its relative magnitude evaluated over the feasible region.

In this paper we first study three conventional methods of scaling: (i) row equilibration followed by column equilibration, (ii) column equilibration followed by row equilibration, and (iii) geometric scaling. Our results indicate that the inconsistent conclusions drawn from different scaling methods arise from the ambiguity in the order of scaling; i.e., row scale followed by column scale versus column scale followed by row scale. Consequently, we design a scaling method, variable normalization and equation equilibration, which does not have this disadvantage. In this method, the variables are normalized so that they obtain the maximum magnitude of 1 over the feasible region. This minimizes their effect on the singular value analysis. The locally linearized equations are then equilibrated so that the maximum term in each equation is of magnitude 1. This places the dominant terms in the equations on the same scale which eliminates numerical problems when evaluating the rank of the system.

Two typical chemical processing units, the continuous stirred tank reactor with a first order endothermic reaction, and a polymerization reactor system are used to demonstrate the singular value method. This approach is implemented as a computer-aided design package.

INTRODUCTION

Recent research and review papers (Ray, 1982; Morari, 1982; Stephanopoulos, 1982; Grossman et al., 1982) have discussed the importance and incentives of increasing the flexibility of chemical plants. For example, having the flexibility to change to different operating conditions when the price of energy changes allows for a more feasible plant operation. Integrating process design, process operation, and process control has been identified as an important step to achieve more flexible systems (Morari, 1981; Stephanopoulos, 1982; Takamatsu, 1982). The variable control structure strategies (Arkun and Stephanopoulos, 1980; Romagnoli et al., 1980; Morari et al., 1980; Govind and Power, 1982; Lau et al., 1985) and the resilient process structure strategies (Lenhoff and Morari, 1982; Marselle et al., 1982; Morari, 1982) can be considered as methodologies designed to provide more flexibility in the plant by either altering the control system or changing the process interconnections. The ultimate goal of these strategies is to increase the performance and the reliability of the system.

The relationship between process control and process design may be represented by different levels. At the lowest level, which is the design of regulatory control structure problem, the measurements, the manipulated variables, and their interconnections are synthesized to regulate the process. Many methods are available for this purpose, ranging from relatively simple criteria such as static relative gain array (Bristol, 1966) and its dynamic extensions (Tung and Edgar, 1977; Witcher and McAvoy, 1977; Gagnepain and Seborg, 1982) to sophisticated computer-aided methods using interactive graphics such as direct Nyquist array (Jensen et al., 1983) and singular value analysis (Lau et al., 1985). The review papers of Ray (1982) and Stephanopoulos (1982) provide comprehensive discussions on this topic. In the industry two methods are commonly used to analyze this problem. In the first approach the control engineer usually designs a control system for a process by using his experience. This approach is heuristic and case-specific. Moreover, when the engineer is confronted with a new or energy-and-material-efficient process, he may need more than his experience and intuition in order to design a satisfactory control system. The second approach is to build a dynamic simulator that is complex enough to capture the essential physical behavior of the system. Different control structures can then be tested by designing a control system for each structure and evaluating its performance. However, a process may have so many candidate control structures that the number of computations becomes prohibitively large.

A variable control structure policy increases the flexibility of the regulatory system because it allows for an adaptive control structure responsive to the effects of the environments and the evolution of the system's structure. However, at the regulatory level the operation of the plant is restricted to a prespecified condition.

The intermediate level of process control/design is the design of changeover control strategy problem, which is the synthesis of control policy taking the process from a current operating condition to the new selected operating condition. It has been addressed in different forms such as steady-state optimizing control (Arkun and Stephanopoulos, 1982a), on-line optimizing control (Bamberger and Isermann, 1978; Prett and Gillette, 1980; Garcia and Morari, 1981), and start-up control policy (Kao, 1980; Brooks, 1979; Han, 1970). In each case, two structural decisions are considered. First, the optimal operating condition is selected. Second, the changeover route (operating route), which may be a sequence of set-point changes or a predesigned trajectory through the feasible region of the process, is synthesized. The common decision variables for the changeover problem are the economics and the stability of the system. Industrial practice for designing changeover policy is a combination of using the process engineer's experience and simulating the dynamics of the process. This design problem is more complicated than the regulatory problem since the nonlinearities of the system and its interconnections must be included in the simulation of the process and in the synthesis of the changeover policy. The changeover policy creates a more flexible response of the system to its surrounding by allowing alternative operating points to be considered. Consequently, the plant is no longer required to operate at a prespecified point. We shall examine in detail the synthesis and selection of a feasible route to implement the changeover policy.

The highest process control/design level is the design of flexible process structures. Here the interconnections between different process units in the plant can be altered to achieve flexibility, operability, and controllability. The primary goal is to integrate process structural design and process control, whereas in the intermediate level we attempt to integrate process parameter design and process control. The task is to select from a number of alternative process configurations one which is the most economically attractive, highly flexible, easily operable and controllable. Morari and his coworkers (Lenhoff and Morari, 1982; Marselle et al., 1982; Morari, 1982, 1983; Morari et al., 1983) have investigated this problem extensively. Their approaches range from multiobjective optimization (Lenhoff and Morari, 1982) where the conflicts between the various objectives of designing a flexible process are examined, to singular value analysis which provides convenient quantitative measures for assessing dynamic sensitivity and invertibility of the system. In the industry, the design engineer assesses the steady-state operability of the plant during the preliminary design stage. However, the control system and its implementation are usually left as an independent design task for the control engineer to perform. It is clear that selecting a flexible process structure improves the operability of the plant, since it now responds better to changes in its surroundings; for example, compensating the effects of disturbances and smoothing out process noises.

As one progresses up the hierarchy of process control and design, the flexibility of the system increases. At the lowest level we can change the manipulated variables, the measured variables, and their interconnections to improve the performance of the control system. However, the operating condition is prespecified and the process structure is fixed. In fact, the primary task of the controller is to keep the process at the designed operation. At the intermediate level, the operating condition is allowed to vary in response to the effects of the environment. In the extreme case where altering the regulatory control structure and the operating condition are no longer sufficient to counter the interactions between the plant and its surrounding, the top level allows the flexibility of altering the process structure to handle such events. There is an encouraging trend in process control research toward improving our understanding of process behavior by using system theory and computer-aided methods to analyze and synthesize control systems and process structures. The insights gained by these studies contribute to a fundamental approach to structural designs.

CHARACTERISTICS OF THE CHANGEOVER POLICY

In this paper we develop a fundamental approach for evaluating changeover policies for a single process unit. The basic motivation behind our methodology stems from the need to balance economic and process control considerations when altering operating conditions in response to changes in the operating environment. The analysis of changeover policies is here done for processes that have a fixed process structure but not necessarily fixed equipment sizes. Varying equipment sizes may be included as parameters in the analysis.

The economic objective function can be evaluated over the feasible region of the process, i.e., the operating region which is bounded by the process constraints (e.g., maximum reactor temperature, maximum vessel volume and pressure) and defined by process equations (mass, energy, and momentum balances on the process unit). Economic contours can be drawn over this feasible region, and the most profitable point is usually at an intersection of constraints (Arkun and Stephanopoulos, 1980; Lee and Weekman, 1976; Webb, 1980). System control measures such as sensitivity and invertibility, concepts which we shall discuss later, also change over the feasible region. Consequently, sensitivity and invertibility contours can be plotted over the feasible region. Comparisons of the contours from the two cases then allow us to balance economic performance with ease of control in the design of a changeover policy. Our task is to develop the proper quantities which measure sensitivity and invertibility. We shall show that singular value analysis of the appropriate system matrix will provide these two measures for our purpose.

This approach has a number of advantages. Since effective numerical algorithms exist for calculating singular value decomposition, computational efficiency is ensured. The system control measures determined by using singular value analysis have single-input single-output analogs. They are relatively simple to understand and have practical appeal. Besides enabling us to simultaneously consider economic performance and controllability in the selection of a new operating point, the approach allows us to avoid using an operating route with controllability problems since it provides information on the controllability of the system over the feasible region.

Singular value analysis has rapidly become a useful design tool in process control and process design because of its simplicity and intuitive appeal. Recently many papers have appeared in the literature investigating applications of this analysis to different problems in process control and design (Doyle, 1981; Morari, 1982; Lau et al., 1985). However, the singular values depend on the scaling of the system, i.e., the physical dimensions which are used in defining the variables and the equations. Consequently, we have to analyze the effects of the scaling of the system on our results. We also need to devise a proper scale so that intrinsic system properties are exposed without being confounded by numerical artifacts.

This problem has been noted (Morari, 1982) but no attempts have been made to systematically explore its implications. In order for singular value analysis to achieve its full potential as a design tool for flexible chemical processes, this question must be considered.

PROBLEM FORMULATION

The operation of a chemical processing unit is constrained by existing process technology, e.g., maximum vessel temperature and

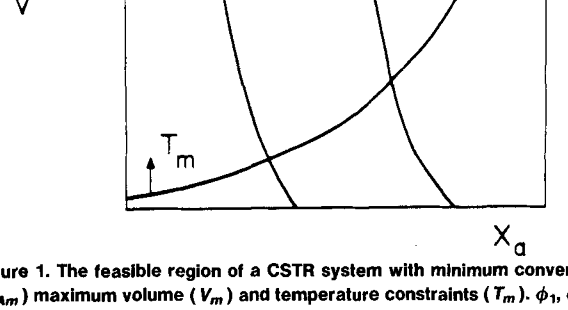

Figure 1. The feasible region of a CSTR system with minimum conversion, (X_{Am}) maximum volume (V_m) and temperature constraints (T_m). ϕ_1, ϕ_2, ϕ are objective function contours. V and X_A are the state variables, volume and concentration, respectively.

pressure, and by mass and energy conservations. For steady-state operation, which is the common mode of operation for a chemical process, these constraints may be modeled by the following algebraic equations:

$$f(x,u,p) = 0 \quad (1)$$

$$h(x,u,p) \leq 0 \quad (2)$$

where dim $x = n_x$, dim $u = n_u$, dim $p = n_p$, dim $f = n_f$, and dim $h = n_h$. Equations 1 and 2 define a feasible operating region for the process. For example, the feasible region for a continuous stirred tank reactor (CSTR) is shown in Figure 1. Since the parameter vector p is a set of variables for Eqs. 1 and 2, the feasible region changes if any element of p changes.

The incentive for designing, constructing, and operating a chemical process lies in its profitability, which may be evaluated by the economic objective

$$\text{Max } \Phi(x,u,p) \quad (3)$$

subject to Eqs. 1 and 2.

Over the feasible region economic contours can be drawn by using Eq. 3 as exemplified in Figure 1. For this example, the maximum lies at the intersection of the temperature and volume constraints.

A changeover control strategy is needed to bring the process to the selected operating condition whenever a low-frequency disturbance such as catalyst deactivation or feedstock change occurs with a large economic impact. It is also needed during start-up once a chemical process reaches its nominal operation. The decision variables in developing this policy have been economic evaluations (Arkun and Stephanopoulos, 1980b; Garcia and Morari, 1980; Prett and Gillette, 1980) as well as heuristic considerations (Arkun and Stephanopoulos, 1980a). When the changeover control policy is implemented, the process moves continuously in the feasible region or along different process constraints. Consequently, the system control measures, sensitivity, and invertibility, also change (Figure 2). These two quantities indicate the controllability of the system at different operating points and thus should be valuable in designing a flexible control strategy.

In subsequent sections we shall demonstrate that singular value analysis of the system matrix provides measures which quantify sensitivity and invertibility. This system matrix depends on the steady-state conditions. Consequently, sensitivity contours and invertibility contours can also be plotted over the feasible region for simple process units so that system control properties can easily be visualized.

SINGULAR VALUE ANALYSIS OF SYSTEM MATRIX

Many sources in the literature describe the mathematical foundation (Noble and Daniel 1977; Forsythe et al., 1977) and the physical interpretations (Weber and Brosilow, 1972; Morari, 1982; Lau et al., 1985) of singular value analysis. Essentially, it allows us to express a general matrix in terms of a dyadic expansion or three decomposition matrices, as in Eq. (4)

$$S_m = Z\Lambda V^{+} = \sum_{i=1}^{r} \sigma_i z_i v_1^{+} \quad (4)$$

where rank $S_m = r$

$$Z = [z_1 z_2 \ldots z_r z_{r+1}]$$

$$V^{+} = [v_1^{+} v_2^{+} \ldots v_r^{+} v_{r+1}^{+}]$$

$$\Lambda = \text{diag}(\sigma_1, \sigma_2, \ldots, \sigma_r, 0)$$

This representation provides the basic structure for our method. In addition to Eqs. 1 and 2 which define the feasible region of the process unit, there exists a third important set of system equations, namely, the measurement equations,

$$y = g(x,u,p) \quad (5)$$

where dim $y = n_y$.

The three sets of equations, Eqs. 1, 2, and 5, combine to provide a mathematical model which approximates the behavior of the process and furnishes information concerning the system. We shall demonstrate how controllability information can be extracted from these equations by using singular value decomposition.

We first define, for convenience, the set X which is the symbolic equivalent to the feasible region given by Eqs. 1 and 2. For any point $(x^*,u^*,p^*)\varepsilon X$, we can calculate the matrix

$$S_m = \begin{bmatrix} A & B \\ C & D \end{bmatrix} \quad (6)$$

where

$$A = \left.\frac{\partial f}{\partial x}\right|_{(x^*,u^*,p^*)}$$

$$B = \left.\frac{\partial f}{\partial u}\right|_{(x^*,u^*,p^*)}$$

$$C = \left.\frac{\partial g}{\partial x}\right|_{(x^*,u^*,p^*)}$$

$$D = \left.\frac{\partial g}{\partial u}\right|_{(x^*,u^*,p^*)}$$

Note that $D = 0$ for most systems, since the measurements rarely are influenced by the manipulated variables. The matrix S_m is the steady-state version of the system matrix defined by Rosenbrock (1970). It provides an internal description of the system locally about the point (x^*,u^*,p^*). Here we analyze the singular values of this steady-state system matrix S_m. The ratio of the maximum singular value σ^* and the minimum one σ^*, the condition number of S_m, $\gamma(\equiv\sigma^*/\sigma_*)$ is a sensitivity measure of the system to any parameter perturbation. The minimum singular value σ_* is a measure of rank deficiency or colinearity in the system and thus also a measure of invertibility. Therefore, σ_* may be interpreted physically as an indicator of control effort. If sufficient points in the set X are analyzed, we can plot sensitivity (γ) and invertibility (σ_*) contours over the feasible region, as illustrated in Figure 3. By combining these results with the economic analysis, we can design a flexible changeover control policy.

STRUCTURAL CONTROLLABILITY AND SINGULAR VALUE ANALYSIS

Morari and Stephanopoulos (1980) have shown that a system represented by a state matrix A, with measurements and manipulated inputs represented by the matrices C and B, is structurally feedback controllable if and only if the two following conditions are satisfied:

(i) (A,B) is structurally controllable

(ii) Generic rank of $S_m = n_f + n_y$

The first condition is obvious and necessary for any control structure. The second condition is interesting and deserves further discussion. Its implications are related to our methodology.

For the rank of S_m to be equal to the number of state and measurement equations, the number of manipulated inputs must be at least as great as the number of measurements. This is an intuitively obvious result if one desires to design a set of feedback loops linking each measurement with each manipulated variable. By inspecting Eq. 4 we see that the above condition is equivalent to the statement that the number of nonzero singular values must be equal to the number of measurement and state equations. Consequently, if the minimum singular value, σ_*, is close to zero, the system may not satisfy condition (ii) and the system matrix cannot be inverted. In any case, a feedback control system designed with this particular control structure will have serious control problems. Morari (1977) provided two other interpretations for condition (ii). It checks the ability of different control actions to achieve a certain steady state. Again we recognize that the singular values provide a measure for the ease of different control structures in achieving the desired steady state. It is a fact well known by the numerical analyst that large a condition number γ (high sensitivity) of the system implies that small perturbations in the system may cause large deviations in its response. The condition (ii) may also be considered equivalent to the condition of functional controllable (Rosenbrock, 1970).

EXTENSION OF THIS METHODOLOGY TO DYNAMIC ANALYSIS

Equation 6 defines the steady-state version of the matrix. Its dynamic version is

$$\begin{bmatrix} A - sI & B \\ C & 0 \end{bmatrix} \tag{7}$$

Singular value analysis of a transfer function matrix has been applied in related works (Morari, 1982; Lau et al. 1985) and presents no conceptual difficulties. Including an interaction measure (as defined by Lau et al., 1985) in our methodology also poses no special problem. However, the inclusion of dynamics and interactions adds to the computational cost and may not always be needed in evaluating changeover policies. Fortunately, we can use the steady-state analysis as a preliminary screening tool to identify critical points in the feasible region, e.g., intersections of constraints. The dynamic and interaction analysis can then be studied for these critical points.

EFFECTS OF SCALING

Scaling, as was mentioned earlier, affects the singular values. This procedure is equivalent to pre- and post-multiplying the system matrix by diagonal matrices in which the elements are scaling factors. By choosing an appropriate scaling method the condition number of the scaled system may be reduced from the original value. If control properties are invariant system properties, then properly scaled variables and equations should allow singular values to correctly predict the behavior of the physical system. It should be stressed that no optimal scaling method exists for a general matrix defined on a vector space with an euclidean norm (Bauer, 1963). Numerous empirical and semiempirical scaling methods have been used successfully by numerical analysts and engineers to solve systems of linear and nonlinear algebraic equations (Forsythe and Moler, 1967; Himmelblau, 1972; Tomlin, 1975; Gill et al., 1981). We will discuss some of these methods and analyze selected examples. As a consequence, we shall demonstrate that the scaling of the variables and equations can drastically change the contours of sensitivity and invertibility. This, in turn, affects the results of the singular value analysis. Furthermore, this treatment will help us to devise a scaling method which is physically appealing for our purpose.

EMPIRICAL METHODS OF SCALING

A simple scaling method is the equilibration method (Forsythe and Moler, 1967). It is very effective in helping to solve systems of algebraic equations. The idea is to scale the variables and equations so that the maximum entry in each row and in each column of the system matrix is of the same magnitude. The equilibration method may significantly reduce the condition number of the matrix. Unfortunately, the major disadvantage of this method is that the order of scaling, row scale followed by column scale or column scale followed by row scale, can affect the result drastically. Our examples will show this fact clearly.

An alternative popular method is the geometric scaling method. An outline of this approach is given by Gill et al. (1981). The basic concept is to scale each row (column) by the geometric mean of its largest and smallest elements. Again the order of scaling affects the results. A combination of the equilibration and geometric scaling methods has also proven effective (Forsythe and Moler, 1967).

Since these are only empirical methods, it is not surprising to find that each method may lead to a different conclusion. Consequently, we have to be extremely careful in order to ensure that our result reflects intrinsic system behavior. A physical understanding of the system is vital. It is only by using both the theoretical approach and our process understanding, that we can reliably design flexible systems.

SEMIEMPIRICAL SCALING METHODS

Tomlin (1975) has observed that a matrix is "well scaled" if the variability of the entries in the matrix is minimal. This observation has led to development of an algorithm which calculates scaling factors so that measures of variability are minimized. Another method (Lau, 1982) based on the observation that the condition number is a measure of the linear dependency of the rows and columns of the matrix calculates scaling factors which minimize an index of linear row and column dependence. These semiempirical methods are useful because they provide scaling factors which minimize certain measures of optimality and have physical interpretations.

SCALING METHOD FOR DESIGNING CHANGEOVER CONTROL STRATEGY

Ideally, the system should be scaled in such a manner that the singular values are truly indicative of its behavior. This should be accomplished by removing the numerical artifacts arising from improper dimensioning of variables and equations. We shall present such a scaling method, which is supported by physical arguments.

The method first limits the variability of the system variables. It then scales the equations so that the maximum terms in the equations are of the same magnitude. By making the variables of the same order of magnitude, we have effectively taken out the numerical effects of "sensitive" variables on the singular value analysis. This procedure is also known as normalization of variables. Scaling the equations so that they have the same magnitude removes the effects of defining an improper physical dimension for the equations. As we shall see subsequently, this scaling method allows us to obtain consistent physical interpretations in the behavior of our examples. Furthermore, the method eliminates the ambiguity in the order of scaling as the major disadvantage of the empirical methods. To illustrate this method, let us consider a CSTR system where a second order reaction $A \xrightarrow{k_1} B$ occurs. For demonstration purposes, we shall consider the material balance only, Eq. 8.

$$f(F, x_A) = \frac{F}{V}(1 - x_A) - k_1 x_A^2 = 0 \tag{8}$$

x_A is the mole fraction of A in reactor, and F is the flowrate of inlet and outlet streams. Suppose that x_A is constrained to be less than 0.7. Rearranging Eq. 8 we can express F as

$$F = k_1 V \frac{x_A^2}{1 - x_A} \tag{9}$$

Consequently, the maximum value which F can attain for the allowable values of x_A is

$$F^* = k_1 V \frac{0.49}{0.3} \cong 1.6\, k_1 V$$

Since x_A is scaled already we need not to find x_A^*. Eq. 8 now can be rewritten as

$$\frac{F^*}{V} q(1 - x_A) - k_1 x_A^2 = 0 \tag{10}$$

$$q = F/F^*$$

The 2×2 system matrix S_m is

$$S_m = \begin{bmatrix} \partial f/\partial x_A & \partial f/\partial q \\ 1 & 0 \end{bmatrix} \tag{11}$$

$$= \begin{bmatrix} -\left(\frac{F^*}{V} q + 2k_1 x_A\right) & \frac{F^*}{V}(1 - x_A) \\ 1 & 0 \end{bmatrix} \quad (12)$$

Combining Eqs. 10 and 11 we obtain

$$S_m = \begin{bmatrix} k_1 x_A \left(\frac{2 - x_A}{1 - x_A}\right) & \frac{F^*}{V}(1 - x_A) \\ 1 & 0 \end{bmatrix} \quad (13)$$

The system matrix, as written in Eq. 13, is normalized. It remains necessary to equilibrate the equations. For the first row we can have two different cases. If $|F^*/V(1 - x_A)| > |k_1 x_A(2 - x_A)/(1 - x_A)|$, the scaling factor is $|F^*/V(1 - x_A)|$. Otherwise, the scaling factor is $|k_1 x_A(2 - x_A)/(1 - x_A)|$. The second row is naturally equilibrated and needs no further considerations. The scaling method may be summarized as:

(1) Find $x_i^* = \text{Max } x_i$

$$\text{s.t. } f(x,u,p) = 0, \quad h(x,u,p) \leq 0 \qquad i = 1, \ldots, n_x$$

(2) Find $u_i^* = \text{Max } u_i$

$$\text{s.t. } f(x,u,p) = 0, \quad h(x,u,p) \leq 0$$

(3) Redefine normalized variables

$$\bar{x}_i = x_i/x_i^*$$
$$\bar{u}_i = u_i/u_i^*$$

and use these variables in calculating the system matrix S_m.

(4) Row equilibrate the system matrix at points of the feasible region and carry out the singular value decomposition. The sensitivity (γ) and invertibility (σ_*) contours may then be plotted.

EXAMPLES

In this section we demonstrate our approach with two typical chemical processes: (1) an endothermic reaction in a continuous stirred tank reactor, and (2) a continuous flow polymerization reactor. These examples are selected because each one exhibits different behavior which demonstrates the usefulness of our approach.

Continuous Stirred Tank Reactor

Arkun (1979) used a first-order endothermic reaction in a CSTR to illustrate the steady-state optimizing control strategy for a single chemical processing unit. Here we analyze a more general form of the same example by using the dimensionless equations given by Ray and Hastings (1980). The CSTR can be modelled by a set of three differential equations.

$$\frac{dx_1}{dt} = q - 1 \quad (14)$$

$$\frac{dx_2}{dt} = -\frac{qx_2}{x_1 + \bar{V}_{M_0}} + \frac{x_1}{x_1 + \bar{V}_{M_0}} Da \exp\left\{\frac{x_3}{1 + x_3/\Gamma}\right\}(1 - x_2) \quad (15)$$

$$\frac{dx_3}{dt} = \frac{(1-\beta)(x_3 + \Gamma)}{\beta}\frac{(q-1)}{x_1 + \bar{V}_{T_0}} - \frac{qx_3}{\beta(x_1 + \bar{V}_{T_0})} + \frac{x_1}{x_1 + \bar{V}_{T_0}} B\, Da \exp\left(\frac{x_3}{1 + x_3/\Gamma}\right)(1 - x_2) + \frac{\bar{Q}_H}{x_1 + \bar{V}_{T_0}} \quad (16)$$

The definitions and the values of the parameters are given in Table 1. This example has two measured variables, the volume and the temperature of the reactor. The two manipulated variables are the feed flow rate and the heating rate. Using Eqs. 14–16 and the measured variables, the 5 × 5 system matrix S_m defined by Eq. 6 can be calculated for different points in X. The economic objective function is chosen as:

$$\Phi = 200\, qx_2 - 3.456\bar{Q}_H \quad (17)$$

TABLE 1. PARAMETERS, EQS. 14–16

x_1	$= \frac{V}{V_{Max}}$	
x_2	$= \frac{C_{Af} - C_A}{C_{Af}}$	
x_3	$= \frac{T - T_f}{T_f}\left(\frac{E}{RT_f}\right)$	
q	$= F_f/F_0$	(1.0)
$\bar{V}_{M_0}$	$= \frac{V_{M_0}}{V_{Max}}$	(1.0)
$\bar{V}_{T_0}$	$= \frac{V_{T_0}}{V_{Max}}$	(2.0)
Da	$= k_0\tau \exp(-\Gamma)$	(0.1)
Γ	$= E/RT_0$	(20.0)
β	$= \frac{(\rho C_p)_T}{\rho C_p}$	(2.0)
τ	$= V_{Max}/F_0$	
B	$= \Gamma\frac{(-\Delta H)C_{Af}}{(\rho C_p)_T T_f}$	(−4.2)
$\bar{Q}_H$	$= \frac{\bar{Q}_H \gamma}{F_0(\rho C_p)_T T_f}$	

The first term in the right hand side of Eq. 17 represents the product revenue and the second term is the cost of providing heat for the reaction. In this example we analyze the economic and controllability contours for $x_1 \varepsilon$ [0.05, 1.0] and $x_2 \varepsilon$ [0.4, 0.99]. In a practical situation there usually is a maximum temperature constraint so that a portion of this region is eliminated (Arkun, 1979). Figures 2a, b, and c show the contours for invertibility, sensitivity, and economic objective, respectively. By comparing these plots we see that the economic performance of the unit is in conflict with the controllability of the system. Optimal economic performance, which in this case, occurs at high volume and conversion, results in high sensitivity γ and poor invertibility (low σ_*) indicating the need for large control efforts. The sensitivity is very high over the entire feasible region. However, the reaction is endothermic so we would expect the reactor to be relatively easy to control, except perhaps at some critical region. Another observation is that the sensitivity and invertibility both predict the same trend. Consequently, we need only to study the sensitivity plot in order to arrive at conclusions regarding controllability for this example.

In Figure 3 we plot the sensitivity for three empirical scaling methods: (i) equilibration (row scale followed by column scale); (ii) equilibration (column scale followed by row scale); (iii) geometric scale (row scale followed by column scale). Immediately, we observe that the order of vector scaling, row scale followed by column scale, or column scale followed by row scale, affects the contours profoundly. The conclusions which we can derive from the various methods differ markedly. For example, the sensitivity plot of the empirical method (ii) indicates that at low volume the sensitivity of the system decreases, as one starts from low conversion, reaches a minimum at some intermediate conversion, and increases again at high conversion. However, the sensitivity plot of empirical method (i) shows that the sensitivity increases with conversion over almost the entire conversion domain. The intricate patterns of sensitivity contours exhibited by the system scaled with method (ii) come about because different entries are used to scale the rows and columns of the matrix over that subregion. Comparison of Figures 3 and 4 shows that the empirical methods are

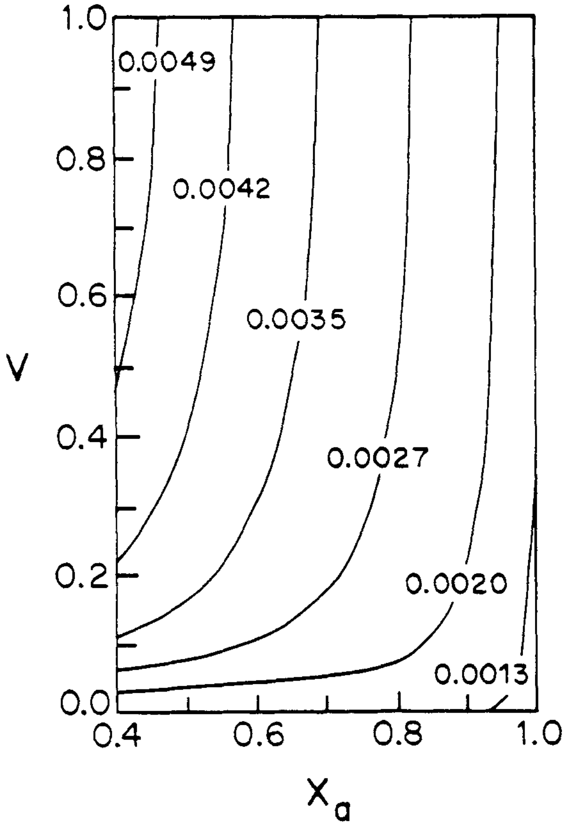

Figure 2a. Invertibility contours for the CSTR system (σ_*).

capable of drastic reduction in the magnitude of the sensitivity as well as in the gradient of the sensitivity over the feasible region. In Figure 2 the sensitivity varies by three orders of magnitude (from 10^4 to 10^7) whereas in Figure 3 the sensitivity for each empirical method changes by less than a factor of 5. Thus, it appears that this system is not particularly difficult to control.

In Figure 4 we show the sensitivity contours of the CSTR scaled by the variable normalization and equation equilibration method. The first striking feature is that over almost the entire feasible region the sensitivity hardly changes. The actual changes are less than a factor of 2. The gradients are steepest in a narrow region of high conversion or low volume. This appeals to our intuition because at high conversion (more energy requirement) or low volume (less material inertia) the system should be more difficult to control. Consequently, in designing a changeover policy, the operating route can be selected easily since controllability poses no problem over much of the feasible region. However, the best operating condition might not be represented solely by the economics, i.e., at conversion greater than 0.95, but rather at conversion closer to 0.9 so as to retain good controllability.

A Continuous-Flow Polymerization Reactor

Brooks (1979) developed a mathematical model for a liquid-phase bulk thermal polymerization reaction of styrene into polystyrene where the polymerization reaction was approximated as a second-order exothermic reaction. He showed that the transient behavior of this system during start-up was very sensitive to variations in initial conditions. Thus, this system is a good candidate for illustrating our approach.

We base our analysis on the following modeling equations:

$$\frac{dx_1}{dt} = -x_1 - \bar{q}(1 - x_1) + Da \exp\left(\frac{x_2}{1 + x_2/\Gamma}\right)(1 - x_1)^2 \quad (18)$$

$$\lambda \frac{dx_2}{dt} = 1 + 2(1 - \bar{q})\frac{\rho S(1 + x_2/\Gamma)}{\rho_0 S_0} DaB \times \exp\left(\frac{x_2}{1 + x_2/\Gamma}\right)(1 - x_1)^2 - \frac{S}{S_0}(1 + x_2/\Gamma) - \bar{Q} \quad (19)$$

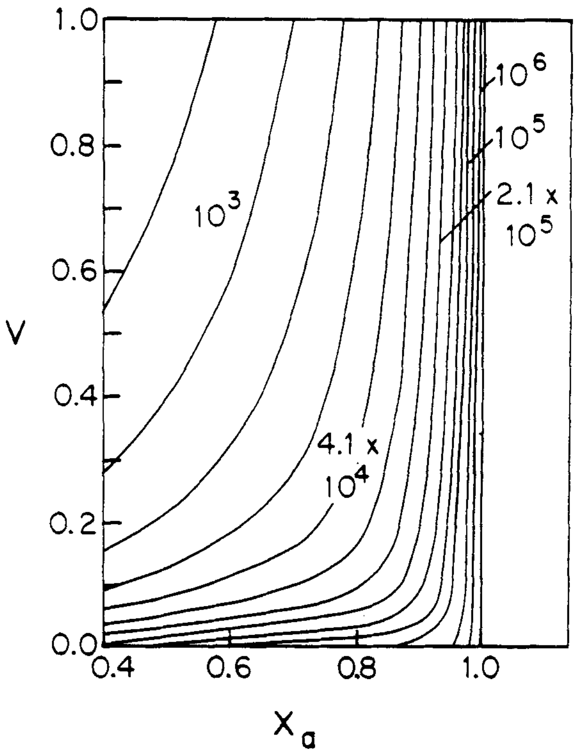

Figure 2b. Sensitivity contours for the CSTR system (γ).

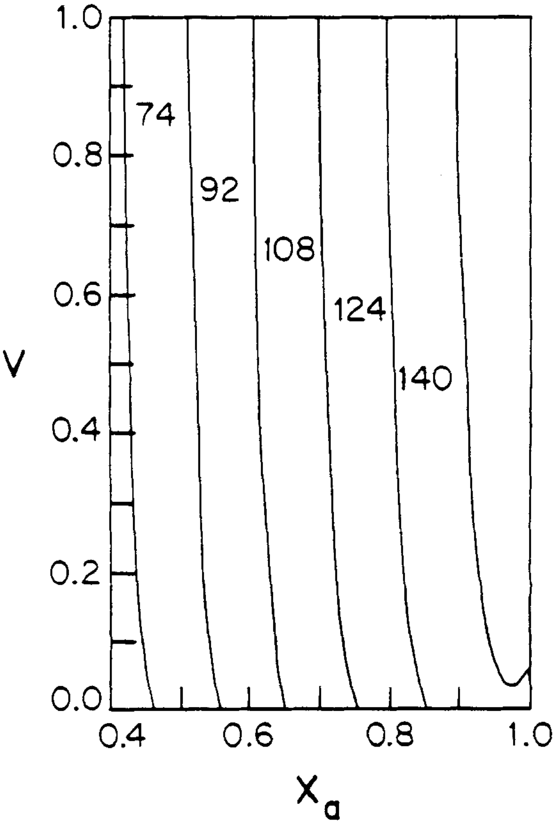

Figure 2c. Economic contours for the CSTR system (Φ).

The definitions and the values of the parameters are given in Table 2. The measured variables are temperature of the reactor and density of the product. The manipulated variables are the inlet and outlet flowrates and the cooling water flowrate. The economic function is for this case

$$\Phi = 195\, x_1 - 5.8\, \bar{Q}_H \quad (20)$$

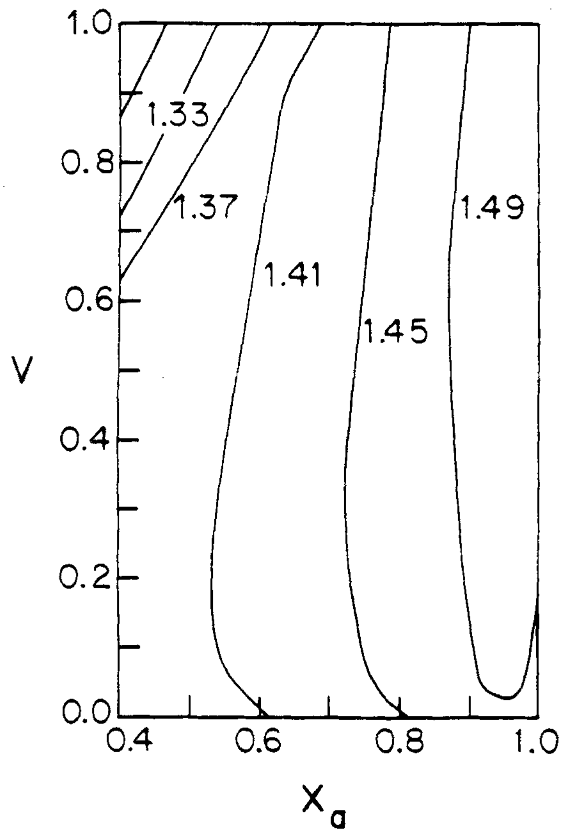

Figure 3a. Sensitivity contours (log γ) for the CSTR system with equilibration by rows followed by columns.

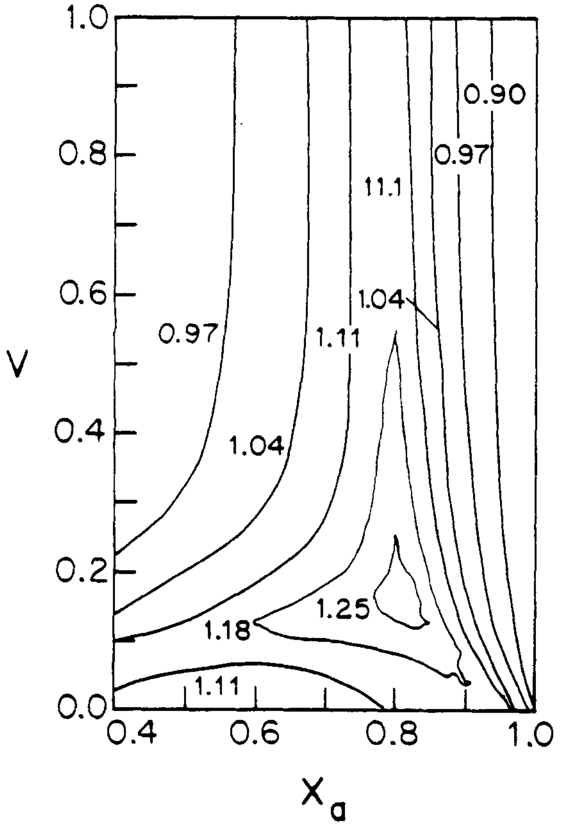

Figure 3b. Sensitivity contours (log γ) for the CSTR system with equilibration by columns followed by rows.

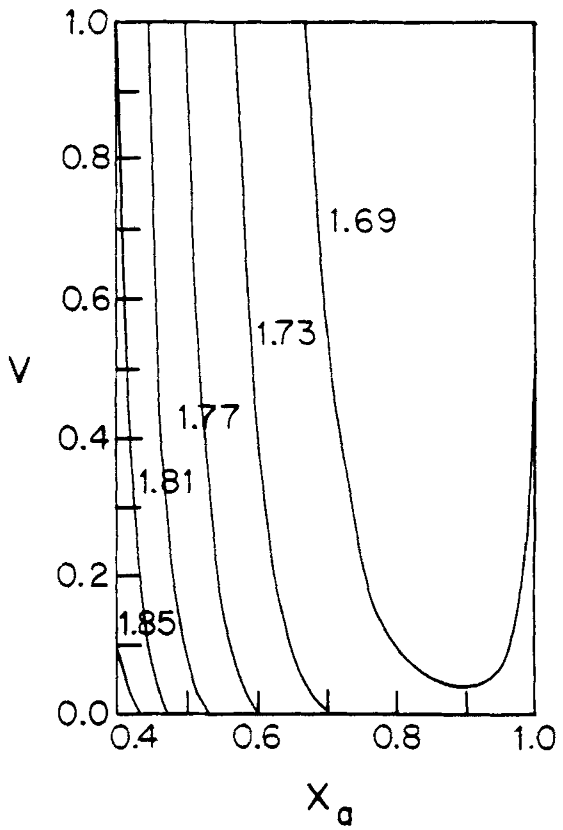

Figure 3c. Sensitivity contours (log γ) for the CSTR system with geometric scaling by rows followed by columns.

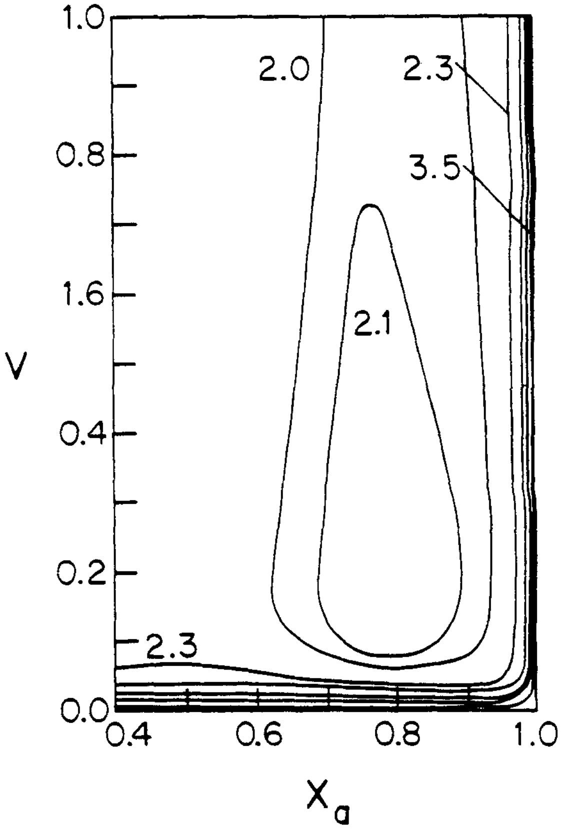

Figure 4. Sensitivity contours (log γ) for the CSTR system with variable normalization and equation equilibration.

TABLE 2. PARAMETERS, EQS. 18–19

x_1	$= \dfrac{C_{Af} - C_A}{C_{Af}}$	
x_2	$= \dfrac{T - T_f}{T_f}\left(\dfrac{E}{RT_f}\right)$	
$\bar{q}$	$= \dfrac{F_f - F_0}{F_0}$	
Da	$= k_0 \tau C_f \exp(-\Gamma)$	(0.1)
τ	$= V/F_0$	
Γ	$= E/RT_f$	(35.0)
ρ	$= n_1 + n_2(1 - x_1) + n_3(1 + x_{2/\gamma})$	
S	$= b_1 + b_2(1 + x_2/\Gamma) + b_3(1 + x_2/\Gamma)^2$	
B	$= \dfrac{(-\Delta H)C_{pf}}{\rho_f S_f T_f}$	(1.225)
$\overline{Q}_H$	$= \dfrac{Q}{F_f \rho_f S_f T_f}$	
λ	$= \left\{\rho T_f(1 + x_2/\gamma)\left[\dfrac{b_2}{\Gamma} + \dfrac{2b_3}{\Gamma}(1 + x_2/\Gamma)\right] + \rho S T_f/\Gamma\right\}/\rho_f S_f T_f$	
C_{Af}	= feed concentration of styrene	
C_A	= concentration of styrene in reactor	
ρ_f	= density of feed (910.9 kg/m^3)	
S_f	= heat capacity of feed (1,752 J/kg/K)	
Tf	= temperature of feed (300 K)	
n_1	= 1,318.7	b_1 = 1,938
n_2	= −150.36	b_2 = −1,131
n_3	= −257.4	b_3 = 945

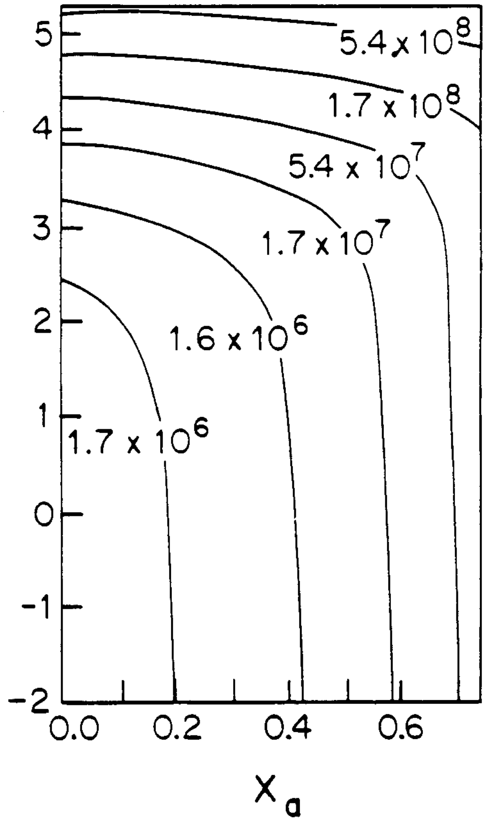

Figure 5b. Sensitivity contours for the polymerization reaction system (γ).

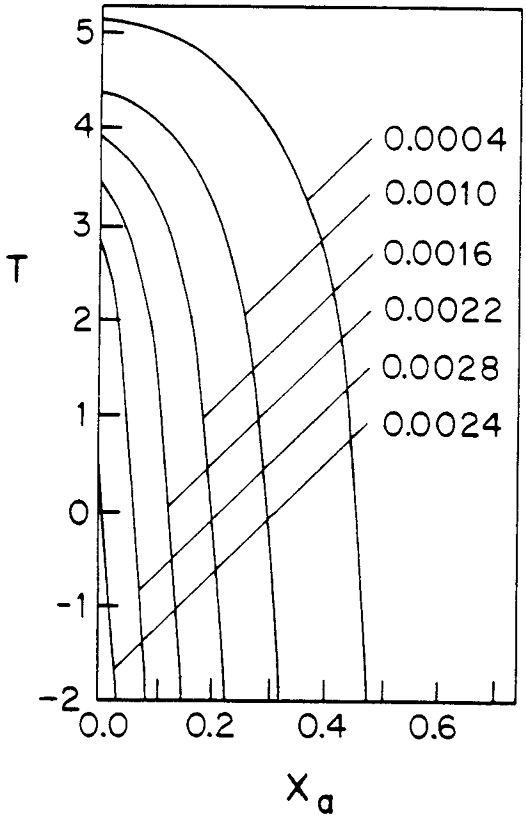

Figure 5a. Invertibility contours for the polymerization reaction system (σ_*).

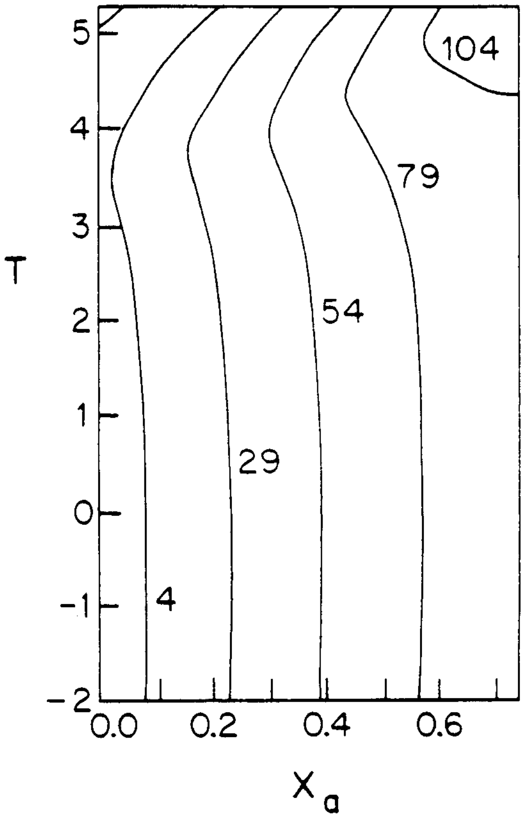

Figure 5c. Economic contours for the polymerization reaction system (Φ).

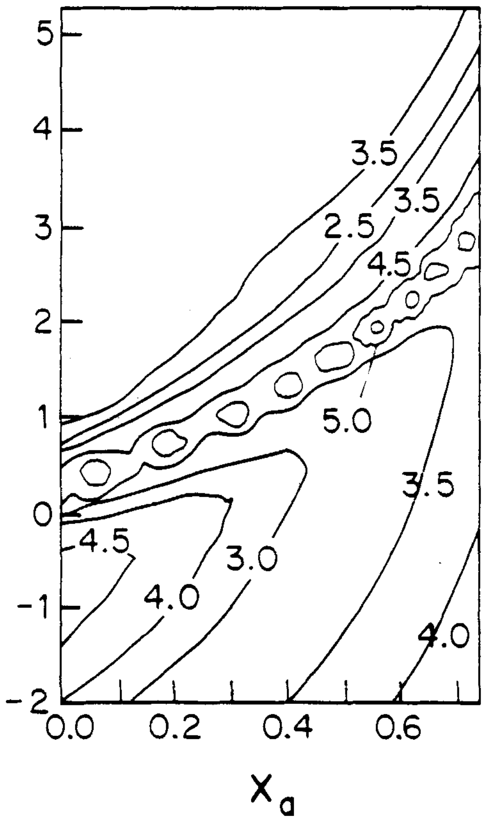

Figure 6a. Sensitivity contours (log γ) for the polymerization reaction system with equilibration by rows followed by columns.

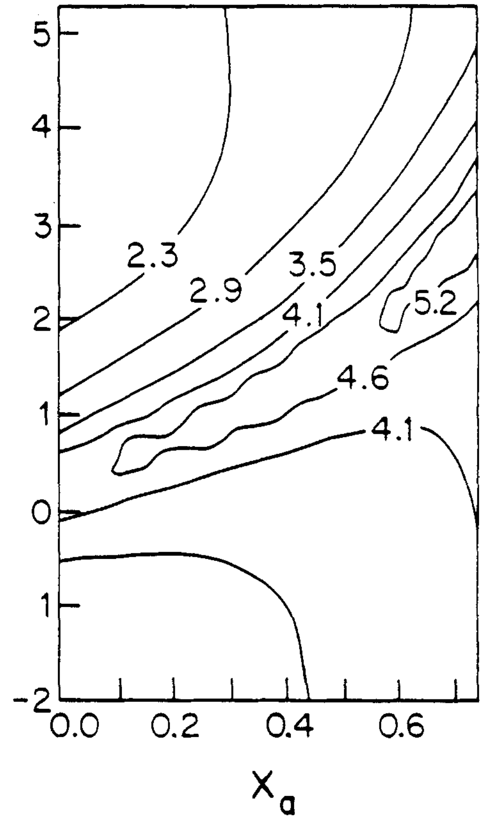

Figure 6c. Sensitivity contours (log γ) for the polymerization reaction system with geometric scaling by rows followed by columns.

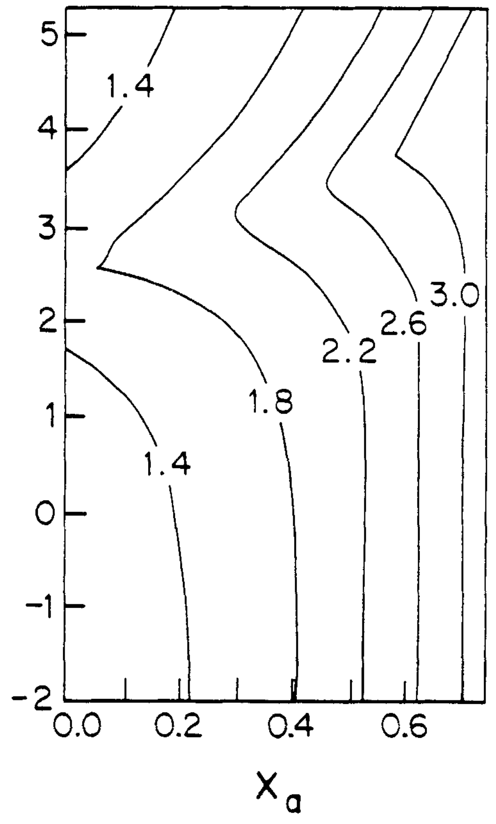

Figure 6b. Sensitivity contours (log γ) for the polymerization reaction system with equilibration by columns followed by rows.

The first term on the righthand side of Eq. 20 is the product revenue and the second term is the cost of cooling the system. The region over which the contours are plotted is $x_1 \varepsilon$ [0.01, 0.7] and x_2 ε [−2.0, 5.0]. This region may contain points which are not practical operating conditions. However, we analyze the behavior of the system over an extended region so that these points are not excluded. Equations (38) and (39), together with the measurement equations, are used to calculate the 4×4 system matrix. The procedure discussed earlier is used to calculate the unscaled sensitivity and invertibility contours in addition to the economic contours. These are shown in Figure 5. Again optimal economic performance is obtained in a region of high conversion and high temperature, where the controllability of the system is poor because of the exothermicity of the reaction. Consequently, it may not always be feasible to operate at the optimal economic point because the system may be more difficult to control. Another striking feature is that at sufficiently high temperature the controllability becomes nearly independent of conversion and increases monotonically with temperature. In Figure 5 the contours are very smooth, contrary to what is observed in Figure 6. The sensitivity contours shown in Figure 6 are scaled by the three empirical methods mentioned earlier and very intricate patterns are observed, particularly for the scaling methods which scale the rows first and then the columns (Figures 6a and b). A ridge extends across the middle of these two plots. This ridge exists because when the rows are scaled first, two equations, the material balance and the density measurement, become nearly linearly dependent in this region. This phenomenon arises purely from the order of scaling; we have no physical explanation for its existence. Another noteworthy point is that the empirical scaling brings down the magnitude of the sensitivity. In Figure 5, the maximum and minimum of sensitivity are approximately 10^9 and 10^6, respectively. In Figure 6 the maximum and minimum are 10^5 and 10^2, respectively. However, in contrast to the CSTR example, large gradients in the sensitivity over the feasible region are not eliminated by scaling. It appears that the system is more difficult to control if it is operated at higher temperature and conversion.

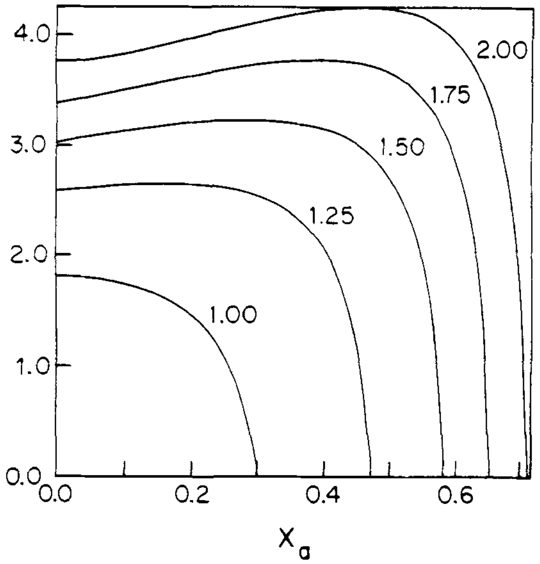

Figure 7. Sensitivity contours (log γ) for the polymerization reaction system with variable normalization and equation equilibration.

Figure 7 shows the sensitivity plot of the system scaled by the variable normalization and equation equilibration method. We plot only a subregion of the feasible regions shown in Figures 5 and 6 because this is sufficient to study the behavior of the system. We have eliminated the intricate patterns which were observed in Figure 6. In fact Figure 7 resembles Figure 5b, except that the magnitude of the sensitivity is much lower, 10^2 as compared to 10^8. But the gradual change in the sensitivity at higher temperature and conversion remains. Consequently, we may choose to operate the system at a suboptimal economic condition in exchange for better controllability. Designing an operating route for the changeover control policy is more difficult because a clear superior route does not exist in any part of the region. In order to go to the region where the profit is high, the operating route will invariably pass through a region of higher sensitivity.

The above examples demonstrate the utility of the singular value analysis in incorporating controllability as well as economic considerations into the design of changeover policies. The methodology relies on having an accurate description of the process in the form of a model, i.e., Eqs. 1, 2, and 5. Therefore, it may be necessary to examine the effects of modeling uncertainties and parameter sensitivity. This can be accomplished by calculating the singular value sensitivity (Freudenberg et al., 1982), which can be derived from perturbation theory. The examples clearly demonstrate the problems associated with finding a proper scaling method. It appears that the variable normalization and equation equilibration approach is suitable for the selection of changeover policies.

The singular value analysis can readily be implemented in a computer-aided design package since the calculations involve straightforward matrix manipulation and eigenvalue calculations. For the same reason the computations are fast. For example, the contours in Figure 7 were determined in less than 1-min CPU (central processing unit) on a Cyber 74. The contour plots are suitable for processes involving changes in two variables such as the two examples presented here, but not for process units or interconnected processes which may require more than two dimensions. The designer will in that case have to make appropriate sections of the parameter space. Future work should extend the presented approach to interconnected, large-scale systems.

ACKNOWLEDGEMENT

Funding for this work came from NSF Grant No. ENG75-11165-A01, the University of Minnesota Computer Center, and the Shell Foundation.

NOTATION

A = linearized state transition matrix
B = linearized input matrix
C = linearized measurement matrix
C_A = concentration of reactant inside reactor
C_{Af} = concentration of feed
E = Arrhenius activation energy
F_f = feed rate
F_o = outlet rate
$-\Delta H$ = heat of reaction
k_0 = Arrhenius reaction rate constant
p = parameter vector
S_m = system matrix
T = temperature inside reactor
T_f = temperature of feed
u = input vector
V = effective volume of reactor
V^+ = right singular value decomposition matrix
V_{max} = maximum effective volume of reactor
V_{M0} = constant mass volume of reactor
V_{T0} = constant thermal volume of reactor
v_i^+ = ith right singlular value decomposition vector
x = state vector
y = measurement vector
Z = left singular value decomposition matrix
z_i = ith left singular value decomposition vector

Greek Letters

γ = condition number
X = feasible region of process
Λ = diagonal matrix of singular values.
σ_i = ith singular values
σ^* = maximum singular values
σ_* = minimum singular values
ρC_p = thermal capacity of reactant
$(\rho C_p)_T$ = thermal capacity of reactor
Φ = economic function

Superscripts

$+$ = transpose and conjugate

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Manuscript received February 18, 1983; revision received November 22 and accepted December 6, 1983.

R & D NOTES

Sedimentation and Fluidization in Solid-Liquid Systems: A Simple Approach

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Because of the interactions among suspension particles, the settling velocity of particles in suspensions is slower than the terminal velocity of a single particle of the same size. The most accurate empirical expression relating the settling velocity to the suspension porosity is represented by

$$U_R = \epsilon^n \quad (1)$$

where U_R is the ratio of the particle velocity relative to the liquid during settling to the terminal velocity of a particle in an infinite medium. (Garside and AlDibouni, 1977) The exponent, n, depends only upon the Reynolds number, (N_{Re}), which is based on the terminal velocity. This expression is similar to the correlation proposed by Richardson and Zaki (1954), although their values of n were slightly different from those of Garside and AlDibouni.

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