Studies in Chemical Process Design and Synthesis

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II. Optimal Synthesis of Dynamic Process Systems with Uncertainty

The concept of the optimal synthesis of dynamic process systems with uncertain parameters is introduced. A structure parameter approach is used to theoretically derive the necessary condition for the optimal performance system structure, and an effective algorithm for implementing the synthesis method is presented. The results are applied to the optimal synthesis of a reactor-separator system for the dynamic start-up of two reaction systems.

SCOPE

Significant progress has been made in the past few years on the synthesis of chemical process systems. The determination of the optimal type and design of processing units, as well as their optimal interconnections within a process flowsheet, can now be done with some success by many synthesis techniques. A good description of the useful techniques has been given by Hendry, Rudd, and Seader (1973), and a latest review of the state of the art of process synthesis can be found in a report by Mah (1975).

One serious limitation with most recent studies of process synthesis is that they are mainly concerned with the synthesis of steady state process systems. A wide variety of important chemical process operations, such as the start-up or shutdown of equipment, the batch or semi-batch operation of processing units, etc., however, fall into the category of dynamic process systems. Furthermore, a large number of recent studies in chemical engineering have shown that certain types of processing units, such as the parametric pumping and the cycling zone absorption, etc., can give better performance by periodic (dynamic) operations. Therefore, it is of practical interest in many situations to consider the problems of dynamics and control at the stage of process synthesis (Mah, 1975; Henley and Motard, 1972) rather than merely synthesizing the process by assuming a steady state operation and then compensating the effect of dynamics by means of control after the synthesis is completed. Unfortunately, except for the recent studies by the authors (Nishida and Ichikawa, 1975; Nishida, Liu, and Ichikawa, 1975*a*), this important aspect of including the dynamics and control considerations in the process synthesis problem has been neglected in the literature. Another important aspect of process synthesis which has not been given sufficient attention is the effect of uncertainty in process parameters. In the literature, only the optimal synthesis of steady state process systems with uncertainty has been studied recently (Nishida, Tazaki, and Ichikawa, 1974).

The objective of this work is to extend the recent results on the optimal synthesis of dynamic process systems (Nishida and Ichikawa, 1975; Nishida, Liu, and Ichikawa, 1975*a*) to include the effect of process parameter uncertainty. The problem considered may be stated briefly as: "Given the process dynamics, how to synthesize the process flow sheet and to specify the process design and control variables subject to the uncertainty in process parameters so as to achieve an optimal dynamic operation of the process?" The approach taken is to consider the synthesis problem as a variable-structure dynamic optimization problem by using the so-called structure parameters. The latter are essentially the splitting factors of process streams connecting various processing units. A number of dynamic process synthesis problems with uncertainty are defined in terms of structure parameters, design and control variables, and uncertain parameters. In particular, the concept of the minimax performance system structure is introduced. This structure will minimize the effect of the worst variations in the uncertain parameters. Both theoretical developments and computational aspects are examined, and illustrative examples are also given.

CONCLUSIONS AND SIGNIFICANCE

This work presents quantitatively several new concepts in the optimal synthesis of dynamic process systems with uncertain parameters. Specifically, the structure parameter approach has been extended to derive theoretically the necessary conditions for several optimal synthesis problems by using the variational calculus. In particular, the optimal set of structure parameters as well as design and control

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variables which will minimize the effect of the worst variations in the uncertain parameters in the minimax structure is presented. An effective computational algorithm for the synthesis of the minimax structure based on the gradient method (Nishida and Ichikawa, 1975; Nishida, Liu, and Ichikawa, 1975*a*) has also been developed. Illustrative examples of the optimal synthesis of a reactor-separator system for the dynamic start-up of two exothermic semibatch reactions are given. Based on both the theoretical and computational results of this work, the following important observations may be stated:

1. In applying the method for the optimal synthesis of dynamic process systems with uncertainty as presented in this work, it is not necessary to include all the process interconnections in the variable-structure dynamic optimization problem in conjunction with the structure parameters. The use of engineering experience or physical insight in determining a restricted system structure for initiating the optimization and the incorporation of an adaptive procedure based on the necessary conditions for the optimal structure for automatically modifying the resulting optimal restricted structures as illustrated in this work will both enhance the successful application of the method for solving high-dimensional dynamic process synthesis problems. For example, an eighth-order dynamic process synthesis problem has been solved requiring only moderate and reasonable computation time and computer storage.

2. Based on the computational results for the two illustrative examples presented, it is concluded that whenever the uncertain parameters have a significant influence on the dynamic behavior of the process to be synthesized, the minimax structure will be quite different from the optimal structure with the nominal values of uncertain parameters. This is illustrated by the important effect of the uncertain inlet molar flow rate ratios of reactants on the process dynamics of an exothermic autocatalytic reaction system. The use of the minimax synthesis is recommended for such situations. On the other hand, if the uncertain parameters do not affect the dynamic behavior of the process significantly, the process structures synthesized based on the nominal values of the uncertain parameters will be similar to those by the minimax method, and thre is no need to use the minimax synthesis. This is also illustrated in an example of the dynamic start-up of an isothermal consecutive reaction system.

PROBLEM FORMULATION

Consider a dynamic process system consisting of (M-2) number of processing units, called subsystems, which convert raw material streams to desired product streams. The dynamic behavior of each subsystem is described by (see Figure 1*a*)

$$\dot{\mathbf{y}}_i(t) = \mathbf{g}_i[\mathbf{y}_i(t), \mathbf{x}_i(i), \mathbf{d}_i, \mathbf{u}_i(t), \mathbf{p}_i, \mathbf{q}_i(t)]$$
$$\mathbf{y}_i(o) = \mathbf{y}_{io} \qquad i = 2,3,\ldots,M-1 \qquad (1)$$

The design and control variables $\mathbf{d}_i$ and $\mathbf{u}_i$ and uncertain parameters $\mathbf{p}_i$ and $\mathbf{q}_i$, which are within their corresponding admissible regions $\mathbf{D}_i$, $\mathbf{U}_i$, $\mathbf{P}_i$, and $\mathbf{Q}_i$, are called the admissible design, control, and uncertain parameters, respectively. For simplicity, the emphasis in the following discussions will be on the single-input and single-output system in which each processing subsystem as well as the whole process system has only one input stream and one output stream. Extensions to the multi-input and multi-output system such as separation units can be learned from the similar formulation for the problem of optimal synthesis of dynamic process systems without uncertainty (Nishida and Ichikawa, 1975; Nishida, Liu, and Ichikawa, 1975*a*) but are illustrated in the later example problems. It is also convenient to use an imaginary input subsystem and an imaginary output subsystem to represent the system input and the system output, respectively. The imaginary input subsystem serves to receive the raw material streams and to distribute them to other subsystems. The imaginary output subsystem collects the output streams of other subsystems and delivers them as the desired product streams to the outside of the process system. No transformation of the state vectors is considered in the imaginary input and output subsystems, and hence

$$\mathbf{y}_i(t) = \mathbf{x}_i(t); \qquad i = 1, M \qquad (2)$$

The structure (flow sheet) of the process system is characterized by a set of structure parameters α_{ij} $(i, j = 1, 2, \ldots M)$ defined by (see Figure 1*b*)

$$\mathbf{x}_i(t) = \sum_{j=1}^{M} \alpha_{ij}\mathbf{y}_j(t), \qquad i = 1, 2, \ldots M \qquad (3)$$

The structure parameters α_{ij} are essentially the splitting fractions of process streams connecting the individual processing units. They are scalar valued variables satisfying the constraints

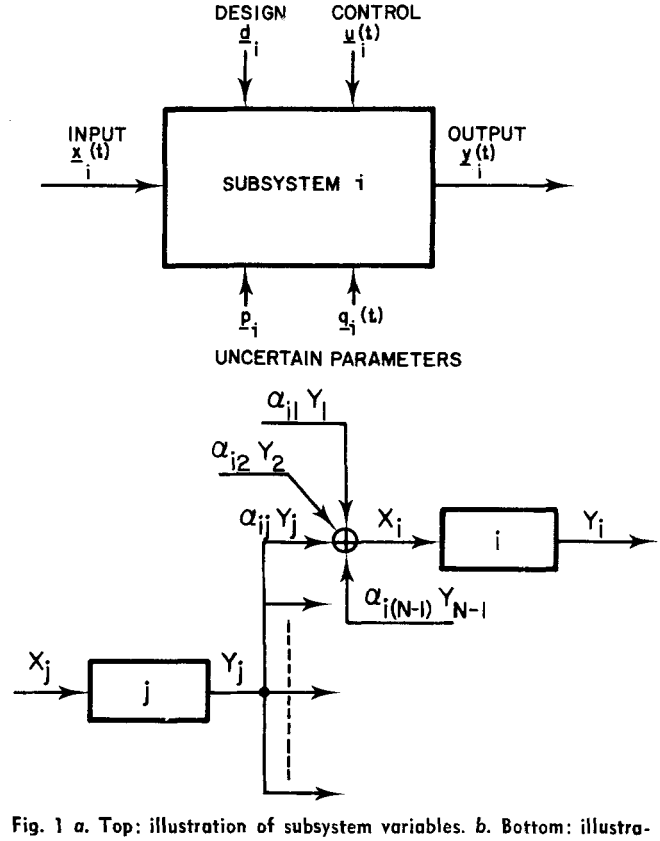


Fig. 1 *a*. Top: illustration of subsystem variables. *b*. Bottom: illustration of system structure and structure parameters.

$$\sum_{j=1}^{M} \alpha_{ij} = 1 \quad (j = 1, 2, \ldots M)$$

$$0 \leq \alpha_{ij} \leq 1 \quad (i, j = 1, 2, \ldots M) \qquad (4)$$

$$\alpha_{1j} = 0 \qquad (j = 1, 2, \ldots M)$$

$$\alpha_{iM} = 0 \qquad (i = 1, 2, \ldots M)$$

As an illustration, in the reactor-separator system shown in Figure 2*a*, α_{31} is the fraction of the feed stream from the imaginary input subsystem 1 which goes to the second continuous stirred-tank reactor (CSTR), subsystem 3. For the multi-input and multioutput subsystem such as the ideal separator (SEP) shown in Figure 2*a*, superscripts may be used to represent different input or output streams; for example, $\alpha^2_{(N+1)4}$ is the fraction of the second output stream from the separator, subsystem 4, which goes to the imaginary output subsystem $N+1$ as the desired product stream. For convenience, the structure parameter matrix with elements α_{ij} $(i, j = 1, 2, \ldots M)$ is denoted by $\boldsymbol{\alpha}$, and the vector $[\alpha_{1i}, \alpha_{2i}, \ldots, \alpha_{Ni}]^T$ is written as $\boldsymbol{\alpha}_{\cdot i}$.

The performance index of the process system to be synthesized, J, is measured by the sum of scalar performance indexes for all processing units or subsystems, J_i $(i = 1, 2, \ldots M)$:

$$J = \sum_{i=1}^{M} J_i$$

$$= \sum_{i=1}^{M} \int_o^{t_f} f_i(\mathbf{x}_i, \mathbf{y}_i, \mathbf{d}_i, \mathbf{u}_i, \mathbf{p}_i, \mathbf{q}_i)dt \qquad (5)$$

Here, the subsystem performance index J_i is the time integral of a given function f_i, which may represent the cost of raw material, the sale of product, the operating cost of the processing unit, etc. This form of subsystem performance index can be considered to be fairly general, since other forms can always be written in this form by defining additional state variables and subsystems.

Based on the above description of the dynamic process system, the synthesis problem may be defined as: "Find the optimal admissible structure parameters α_{ij}, designs $\mathbf{d}_i$, and controls $\mathbf{u}_i$ which satisfy the subsystem dynamics, (1) and (2), to minimize the process performance index, (5), subject to the uncertainty in process parameters." In this study, four types of performance indexes are used which lead to different types of optimal synthesis problems. These are described as follows.

The first problem is to find the optimal values of structure parameters, design, and control variables which will minimize the performance index, (5), when uncertain parameters are specified at their nominal values. The resulting system structure will be called the nominally optimal performance system structure or the nominally optimal structure. Mathematically, this is equivalent to the minimization problem represented by

$$J(\mathbf{v}^o, \mathbf{w}^N) = \min_{\boldsymbol{\alpha},\mathbf{d},\mathbf{u}} J(\mathbf{x}, \mathbf{y}, \boldsymbol{\alpha}, \mathbf{d}, \mathbf{u}, \mathbf{p}^N, \mathbf{q}^N)$$

$$= \min_{\mathbf{v}} J(\mathbf{v}, \mathbf{w}^N) \qquad (6)$$

along with the constraints (1) to (4), where $\mathbf{v} = (\boldsymbol{\alpha}, \mathbf{d}, \mathbf{u})^T$ and $\mathbf{w} = (\mathbf{p}, \mathbf{q})^T$. The solution to this problem has been presented in previous papers (Nishida and Ichikawa, 1975; Nishida, Liu, and Ichikawa, 1975*a*).

The next problem is to find the minimax performance system structure or the minimax structure, which will compensate the effect of the worst variation of uncertain

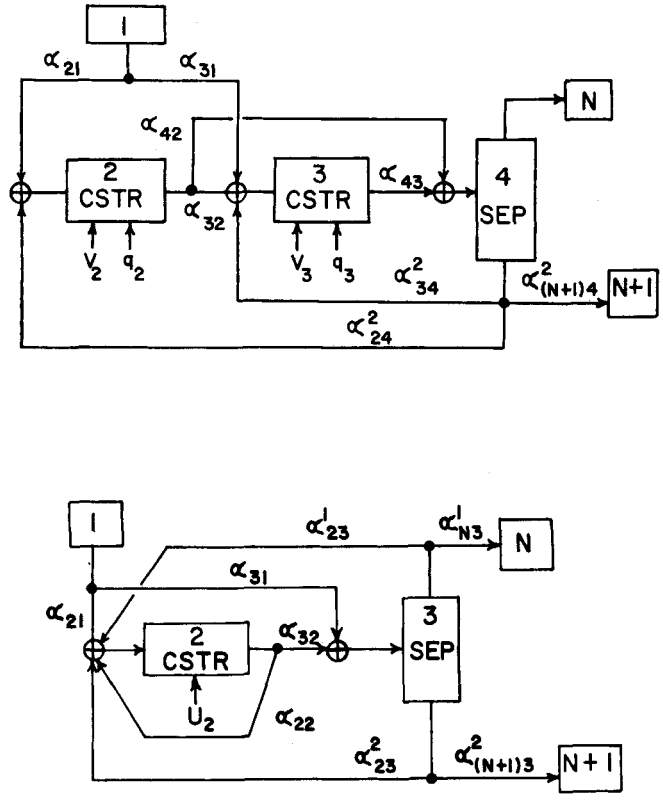


Fig. 2 *a.* Top: initially restricted system structure for example 1. *b.* Bottom: initially restricted system structure for example 2.

parameters by choosing the optimal set of structure parameters, design, and control variables. This can be examined mathematically by first studying the maximum increase in the value of the performance index, (5), caused by the worst variation of uncertain parameters, when structure parameters, design, and control variables are specified at their nominal values. This auxiliary problem can be described by

$$J(\mathbf{v}^N, \mathbf{w}^*) = \max_{\mathbf{p},\mathbf{q}} J(\mathbf{x}, \mathbf{y}, \boldsymbol{\alpha}^N, \mathbf{d}^N, \mathbf{u}^N, \mathbf{p}, \mathbf{q})$$

$$= \max_{\mathbf{w}} J(\mathbf{v}^N, \mathbf{w}) \qquad (7)$$

The system structure defined by (7) will be called the nominal performance system structure with worst uncertain parameters. Here, it is assumed that the upper and/or lower bounds of uncertain parameters can be measured or estimated, and hence

$$\mathbf{p}_i^L \leq \mathbf{p}_i \leq \mathbf{p}_i^U \qquad (i = 1, 2, \ldots m) \qquad (8)$$

$$\mathbf{q}_i^L \leq \mathbf{q}_i(t) \leq \mathbf{q}_i^U \qquad (i = 1, 2, \ldots l) \qquad (9)$$

The minimax structure is then defined by

$$J(\mathbf{v}^o, \mathbf{w}^*) \equiv \min_{\boldsymbol{\alpha},\mathbf{d},\mathbf{u}} \max_{\mathbf{p},\mathbf{q}} J(\mathbf{x}, \mathbf{y}, \boldsymbol{\alpha}, \mathbf{d}, \mathbf{u}, \mathbf{p}, \mathbf{q})$$

$$\equiv \min_{\mathbf{v}} \max_{\mathbf{w}} J(\mathbf{v}, \mathbf{w}) \qquad (10)$$

This minimax approach essentially considers the dynamic process synthesis problem with uncertainty as a differential game (Bryson and Ho, 1969; Ciletti and Starr, 1970) between uncertain parameters and decision variables appearing in the synthesis which consist of structure parameters, design, and control variables. While uncertain parameters attempt to maximize the performance index, the best set of structure parameters, design, and control variables in this worst-case synthesis is to be determined. In an earlier paper (Nishida, Tazaki, and Ichikawa, 1974), this approach was applied to the synthesis of steady state proc-

ess systems with uncertainty, in which further discussions on the minimax synthesis technique were given. A more general treatment of considering the minimax synthesis technique as one of the several possible approaches for the optimal synthesis of process systems with vector-valued or multiple performance indexes can be found in Liu et al. (1976). Here, it is sufficient to mention that although the minimax approach is usually a conservative one, the process system synthesized based on the minimax performance index gives the process designers an assurance that the actual performance of the process system will never be worse than the one calculated from (10).

The last performance index used in this study is $J(\alpha^N, \mathbf{d}^N, \mathbf{u}^N, \mathbf{p}^N, \mathbf{q}^N)$, the nominal performance index. This requires all variables appearing in the performance index (5) to be specified at their nominal values. The corresponding system structure will be called the nominal performance system structure or the nominal structure.

THEORETICAL DEVELOPMENTS

Necessary Conditions for Nominal Performance System Structure with Worst Uncertain Parameters, $J(\mathbf{v}^N, \mathbf{w}^*)$

In order to derive the necessary conditions by means of variational calculus, several assumptions must be made. The functions f_i and $\mathbf{g}_i$ are both twice continuously differentiable and satisfy the Lipschitz conditions. For each subsystem, the output steam state vector $\mathbf{y}_i$ is uniquely determined when the input stream state vector $\mathbf{x}_i$, design vector $\mathbf{d}_i$, and control vector $\mathbf{u}_i$ are given. Also, $\mathbf{u}_i$ is piecewise continuous in the time interval $[0, t_f]$.

It is appropriate to introduce the Hamiltonians H_i^N and S_i^N as

$$H_i^N \equiv -f_i(\mathbf{x}_i, \mathbf{y}_i, \mathbf{d}_i^N, \mathbf{u}_i^N, \mathbf{p}_i, \mathbf{q}_i) + \boldsymbol{\lambda}_i^T \mathbf{g}_i(\mathbf{x}_i, \mathbf{y}_i, \mathbf{d}_i^N, \mathbf{u}_i^N, \mathbf{p}_i, \mathbf{q}_i) \quad (11)$$

$$S_i^N \equiv \sum_{k=1}^{M} \{\mathbf{u}_k^T \mathbf{y}_i \boldsymbol{\alpha}_{\cdot i}^N\} \quad i = 1, 2, \ldots, M \quad (12)$$

where $\boldsymbol{\lambda}_i$ and $\boldsymbol{\mu}_i$ are the adjoint vectors defined by

$$\dot{\boldsymbol{\lambda}}_i + \boldsymbol{\lambda}_i^T \frac{\partial \mathbf{g}_i}{\partial \mathbf{y}_i} - \frac{\partial \mathbf{f}_i}{\partial \mathbf{y}_i} + \sum_{k=1}^{M} \boldsymbol{\alpha}_{\cdot i}^N = 0$$

$$\frac{\partial f_i}{\partial \mathbf{x}_i} - \boldsymbol{\lambda}_i^T \frac{\partial \mathbf{g}_i}{\partial \mathbf{x}_i} + \boldsymbol{\mu}_i^T = 0 \quad i = 1, 2, \ldots, M \quad (13)$$

$$\boldsymbol{\lambda}_i^T = 0$$

The admissible time-independent uncertain parameters $\mathbf{p}_i$ $(i = 1, 2, \ldots, m)$ are said to satisfy the weak minimum condition, if for given values of $\mathbf{x}_i$, $\mathbf{y}_i$, $\boldsymbol{\lambda}_i$, $\boldsymbol{\mu}_i$, $\mathbf{d}_i^N$, $\mathbf{u}_i^N$, and $\mathbf{q}_i$, the time-averaged Hamiltonians

$$\overline{H}_i^N \equiv \int_o^{t_f} H_i^N(\mathbf{x}_i, \mathbf{y}_i, \boldsymbol{\lambda}_i, \mathbf{d}_i^N, \mathbf{u}_i^N, \mathbf{p}_i, \mathbf{q}_i)\, dt \quad (14)$$

$$\overline{S}_i^N \equiv \int_o^{t_f} S_i^N(\mathbf{y}_i, \boldsymbol{\mu}_i, \boldsymbol{\alpha}_{\cdot i}^N)\, dt \quad (15)$$

are either stationary with respect to $\mathbf{p}_i$ or attain their minimum values when $\mathbf{p}_i$ is on the boundary of the admissible region $\mathbf{P}_i$. The time-dependent uncertain parameters $\mathbf{q}_i(t)$ $(i = 1, 2, \ldots, l)$ are said to satisfy the minimum condition if at any instant $t \in [0, t_f]$ the function H_i^N attains its minimum value for given values of $\mathbf{x}_i$, $\mathbf{y}_i$, $\boldsymbol{\lambda}_i$, $\mathbf{u}_i^N$, $\mathbf{d}_i^N$, and $\mathbf{p}_i$. Since the function $\overline{H}_i^N$ is not an explicit function of $\boldsymbol{\alpha}_{\cdot i}$ and $\overline{S}_i^N$ is not an explicit function of $\mathbf{p}_i$, the minimization of the time-averaged Hamiltonians or the weak minimization of $\overline{H}_i^N$ and $\overline{S}_i^N$ can be carried out separately, the former with respect to $\mathbf{p}_i$ and the latter with respect to $\boldsymbol{\alpha}_{\cdot i}$. The following necessary conditions can then be obtained:

"If a system structure of a dynamic process system is the nominal performance system structure with worst uncertain parameters defined by the performance index $J(\mathbf{v}^N, \mathbf{w}^*)$, (7), the admissible time-independent uncertain parameters $\mathbf{p}_i$ $(i = 1, 2, \ldots, m)$ satisfy the weak minimum condition, and the admissible time-dependent uncertain parameters $\mathbf{q}_i(t)$ $(i = 1, 2, \ldots, l)$ satisfy the minimum condition."

Necessary Conditions for Minimax Performance System Structure, $J(v^o, w^*)$

To determine the optimal set of structure parameters, design, and control variables which will minimize the effect of the worst variations in uncertain parameters corresponding to the minimax structure, it is necessary to define several new Hamiltonians H_i, S_i, $\overline{H}_i$, and $\overline{S}_i$. These functions are essentially similar to the preceding ones, H_i^N, S_i^N, $\overline{H}_i^N$, and $\overline{S}_i^N$. Their expressions can be written simply by replacing the nominal values $\mathbf{d}_i^N$, $\mathbf{u}_i^N$, and $\boldsymbol{\alpha}_{\cdot i}^N$ in (11) and (12) and (14) and (15) by $\mathbf{d}_i$, $\mathbf{u}_i$, and $\boldsymbol{\alpha}_{\cdot i}^N$ respectively. The admissible structure parameters and design variables are said to satisfy the weak maximum condition if, for given values of $\mathbf{x}_i$, $\mathbf{y}_i$, $\boldsymbol{\lambda}_i$, and $\boldsymbol{\mu}_i$, the time-averaged Hamiltonians $\overline{H}_i$ and $\overline{S}_i$ are, respectively, either stationary with respect to structure parameters and design variables that lie in the interior of the admissible regions, or attain their maximum values when the admissible structure parameters and/or design variables lie on the boundary of the admissible regions. The admissible control variables are said to satisfy the maximum condition if at any instant $t \in [0, t_f]$ the Hamiltonian H_i attains its maximum value for given values of $\mathbf{x}_i$, $\mathbf{y}_i$, $\boldsymbol{\lambda}_i$, and $\boldsymbol{\mu}_i$. By extending the analysis in the previous papers (Nishida and Ichikawa, 1975; Nishida, Liu, and Ichikawa, 1975*a*, 1975*b*; Nishida, Tazaki, and Ichikawa, 1974), the following necessary conditions can be obtained:

"If a system structure of dynamic process system is the minimax structure, the optimal set of admissible structure parameters, design, and control variables and uncertain parameters $\boldsymbol{\alpha}^o$, $\mathbf{d}_i^o$, $\mathbf{u}_i^o$, $\mathbf{p}_i^*$, and $\mathbf{q}_i^*(t)$, respectively, is at the saddle point of the Hamiltonians H_i and S_i. In other words, the admissible structure parameters $\boldsymbol{\alpha}^o$ and design variables $\mathbf{d}_i^o$ satisfy the weak maximum conditions, and control variables $\mathbf{u}_i^o$ satisfy the maximum condition for given uncertain parameters, while the admissible time-independent uncertain parameters $\mathbf{p}_i^*$ satisfy the weak minimum condition, and the admissible time-dependent uncertain parameters $\mathbf{q}_i^*(t)$ satisfy the minimum condition for given structure parameters, design and control variables." By denoting the weak maximization of A with respect to b under the constraints of B, C, ... as $\underset{b}{w\max}\{A; B, C, \ldots\}$, the weak maximization of $\overline{S}_i$ with respect to $\boldsymbol{\alpha}_{\cdot i}$ can be represented by

$$\underset{\boldsymbol{\alpha}_{\cdot i}}{w\max} \left\{ \int_o^{t_f} \sum_{k=1}^{M} \mu_k^T y_k \alpha_{ki}\, dt; \quad \sum_{k=1}^{M} \alpha_{ki} = 1, \quad 0 \leq \alpha_{ki} \leq 1 \right\} \quad (16)$$

for $i = 1, 2, \ldots, M$. The optimal structure parameters as the solution to (16) are of particular importance in the synthesis of system structure and can be shown to be (Nishida and Ichikawa, 1975; Nishida, Liu, and Ichikawa,

1975*a*, 1975*b*)

$$\alpha_{ki} = 1 \quad \text{if} \quad M_{ki} = \max_l M_{li} \tag{17}$$

$$0 \leq \alpha_{ki} \leq 1 \quad \text{and} \quad \sum_{k=1}^{M} \alpha_{ki} = 1 \quad \text{if} \quad k \in k_i \tag{18}$$

$$\alpha_{ki} = 0 \quad \text{if} \quad k \notin k_i \tag{19}$$

In (17), (18), and (19)

$$M_{ki} = \int_o^{t_f} \mu_k{}^T \, y_i \, dt \tag{20}$$

is called the structure parameter function, and k_i designates a set of subsystem numbers k's for which the corresponding M_{ki}'s are maximum; that is

$$k_i = \{k; \quad M_{ki} = \max_l \quad M_{li}\} \quad \text{for} \quad i = 1, 2, \ldots, M \tag{21}$$

The condition (17) implies that if the output stream of subsystem i, y_i, goes completely to subsystem j as an input stream, that is, when $\alpha_{ji} = 1$, then the value of M_{ki} is the maximum among all M_{ki}'s for $k = 1, 2, \ldots, M$. The condition (18) suggests that if fractions of the output stream of subsystem i, y_i, are fed to different subsystems k's, that is, if $0 \leq \alpha_{ki} \leq 1$ and $\sum_{k=1}^{M} \alpha_{ki} = 1$, then all the subsystems k's which receive y_i as input streams will have the same maximum value of M_{ki}.

Because of space limitations, the solution of other maximization and minimization problems for finding the optimal set of design and control variables, as well as time-independent and time-dependent uncertain parameters in the minimax structure, will not be described here. Interested readers are referred to the similar analysis given in the previous papers (Nishida, Liu, and Ichikawa, 1975*a*, 1975*b*; Nishida, Tazaki, and Ichikawa, 1974).

COMPUTATIONAL ASPECTS

The use of (17) to (19) for specifying the optimal values of structure parameters requires the knowledge of the structure parameter function M_{ki}. The latter depends on the values of adjoint vectors, which are solved from the adjoint equations (13). The adjoint equations, in turn, involve the optimal values of structure parameters to be determined. Fortunately, an iterative procedure such as the gradient method has been shown to be very effective in solving a similar boundary-value problem to obtain the optimal values of structure parameters, design, and control variables (Nishida and Ichikawa, 1975; Nishida, Liu, and Ichikawa, 1975*a*). In this study, in order to enhance the applicability of the gradient method for solving high-dimensional synthesis problems, this method is applied primarily to optimize an initially restricted system structure. Specifically, a restricted system structure is the one in which some of the structure parameters are fixed at preassigned values, possibly at zero, and the rest of the structure parameters, design, and control variables, and uncertain parameters are allowed to vary during the optimization process. The optimal system structure obtained under this initially restricted condition will be called the restricted optimal system structure. Based on the preceding theoretical developments, the true optimality of the restricted optimal system structure when no restrictions on the structure parameters are included can be examined by the magnitude of the structure parameter function. This aspect will be incorporated in the following computational algorithm. For convenience, several notations are first defined here:

$I_i \equiv \{k;\ \alpha_{ki}$ is allowed to vary in the restricted structure$\}$

$\overline{I}_i \equiv \{k;\ \alpha_{ki}$ is fixed at zero in the restricted structure$\}$

$\tilde{I}_i \equiv \{k;\ 1 > \alpha_{ki} > 0$ in the optimal restricted structure$\}$

where $i = 1, 2, \ldots, M$.

A Minimax Structure Algorithm

Step 1. Assume an initially restricted system structure $I_i^{(j)}$ ($i = 1, 2, \ldots, M$, and initially $j = 0$), where the superscript (j) stands for the j^{th} iteration.

Step 2. Assume the initial estimates, $\alpha_{ij}^{(k)}$ (initially $k = 0$), of the admissible structure parameters, where the superscript (k) denotes the k^{th} trial.

Step 3. Solve the problem $\min_{\mathbf{v}} \max_{\mathbf{w}} J$ defined by (10) with the fixed values of structure parameters, $\alpha_{ij}^{(k)}$, (a) guessing $\mathbf{v}_{(r)}$ (initially $r = 0$) in the admissible region, where the subscript (r) stands for the r^{th} trial within the computational routine of step 3; (b) determining the worst uncertain parameters $\mathbf{w}^*$ by solving the problem $\max_{\mathbf{w}} J$ with the fixed $\mathbf{v}_{(r)}$; (c) returning to (a) and repeating the procedure until $J\,[\alpha_{ij}^{(k)}, \mathbf{v}^o, \mathbf{w}^*]$ is obtained.

Step 4. If $J\,[\alpha_{ij}^{(k)}, \mathbf{v}^o, \mathbf{w}^*] = J\,[\alpha_{ij}^{(k-1)}, \mathbf{v}^o, \mathbf{w}^*]$, go to step 6; otherwise go to step 5.

Step 5. Compute the state and adjoint vectors and modify the structure parameters for the $(k+1)^{\text{th}}$ trial by

$$\alpha_{ij}^{(k+1)} = \alpha_{ij}^{(k)} + \epsilon \left(\frac{\partial \overline{S}}{\partial \alpha_{ij}} \right)^{(k)}, \quad (i, j = 1, 2, \ldots, M)$$

where ϵ is a positive step size factor.

Step 6. If all of the computed structure parameters α_{lk} are such that

$$M_{li} < M_{ki}; \quad l \in \overline{I}_i, \quad k \in \tilde{I}_i, \quad i = 1, 2, \ldots, M \tag{22}$$

then the optimal restricted minimax structure satisfies the necessary condition for the optimal structure even when no initial restrictions on the structure parameters are included, and the iterative optimization terminates. If any of the structure parameters α_{lk} is such that

$$M_{li} > M_{ki}; \quad l \in I_i^{(j)}, \quad k \in \tilde{I}_i^{(j)}, \quad i = 1, 2, \ldots, M \tag{23}$$

then l of $\alpha_{li}^{(j)}$ should become a member of $I_i^{(j+1)}$ in the next restricted structure, and all k's of $\alpha_{ki}^{(j)}$ should remain as members of $I_i^{(j+1)}$. Also, all k's of $\alpha_{ki}^{(j)}$ such that $k \in I_i^{(j)}$ and $k \in \tilde{I}_i^{(j)}$ are removed from $I_i^{(j+1)}$.

Step 7. Return to step 2 and repeat steps 2 to 7 until (22) is satisfied.

It should be mentioned that the above computational algorithm may yield only a locally optimal solution to the synthesis problem, depending upon the starting values of the structure parameters, design, and control variables and uncertain parameters. Furthermore, the condition (22) is generally only necessary and not sufficient, except for the linear separable dynamic systems. In order to obtain a global optimum, the iterative optimization has to be tried with different sets of starting values. However, the above algorithm has an advantage in that it is not necessary to include all the possible interconnections among the available processing units or subsystems in the initially restricted system structure in step 1. Even if some of the necessary interconnections are omitted in the initially restricted system structure, the adjustment provided by step 6 in the above algorithm will automatically modify the initial structure properly. Consequently, this

adaptive procedure can greatly enhance the successful use of engineering experience or physical insight in the determination of the initially restricted system structure for the dynamic process system to be synthesized.

ILLUSTRATIVE EXAMPLES

Example 1

Consider a process synthesis problem in which the optimal interconnections of a maximum number of two available continuous stirred-tank reactors (CSTR) and an ideal separator (SEP) as well as the optimal reactor volumes are to be determined for the start-up operation for a first-order reaction $A \xrightarrow{K_1} B \xrightarrow{K_2} C$ Here, A is the raw material, B the desired product, and C the undesired product. Initially, either one or both of the two CSTRs will be filled with an inert fluid D. At time $t = 0$, the start-up of the system is initiated by continuously supplying the reactant A. This is continued for a certain finite time period $[0, t_f]$. The ideal separator removes completely products B and C from the rest of the reaction mixture, A and D.

If it is assumed that the molar volume is the same for all the components and does not change with time during the reaction, the dynamic behavior of the two CSTRs can be written in terms of the molar flow rates of the components as

$$\begin{aligned}
\dot{y}_{iA} &= \frac{1}{\theta_i}(x_{iA} - y_{iA}) - K_1 y_{iA} \\
\dot{y}_{iB} &= \frac{1}{\theta_i}(x_{iB} - y_{iB}) + K_1 y_{iA} - K_2 y_{iB} \\
\dot{y}_{iC} &= \frac{1}{\theta_i}(x_{iC} - y_{iC}) + K_2 y_{iB} \\
\dot{y}_{iD} &= \frac{1}{\theta_i}(x_{iD} - y_{iD}) \\
y_{is}(0) &= y_{is}^{o}
\end{aligned} \tag{24}$$

where $i = 2, 3$ represents the subsystem number for the two CSTRs and $s = A, B, C, D$ denotes the material A, B, C, and D, respectively. x_i is the input molar flow rate to the specified subsystem i and y_i the output molar flow rate. The reaction rate constants K_1 and K_2 are given by $K_1(T_i) = K_{10}\exp(-E_1/RT_i)$ and $K_2(T_i) = K_{20}\exp(-E_2/RT_i)$, where R is the ideal gas constant, T_i $(i = 2, 3)$ is the temperature of the CSTR with the subsystem number i, K_{10} and K_{20} are both constants, and E_1 and E_2 are the activation energy constants. The mean reactor holding time θ_i in (24) is related to the reactor volume V_i to be specified by

$$\theta_i = V_i/(x_{iA} + x_{iB} + x_{iC} + x_{iD})\rho, \quad i = 2, 3 \tag{25}$$

The operating cost of a CSTR per unit time is

$$f_i = aV_i = a\theta_i\rho(x_{iA} + x_{iB} + x_{iC} + x_{iD}), \quad i = 2, 3 \tag{26}$$

where a is the cost factor for the CSTR.

Nominally, the reaction proceeds isothermally in the CSTRs. The temperature fluctuation of the CSTR from the nominal temperature is taken as the uncertain parameter variation, and hence

$$T_i(t) = T_i^N + q_i(t) \quad t \in [0, t_f] \tag{27}$$

The uncertain temperature variation $q_i(t)$ may cause the formation of the undesirable product C and the decrease in the rate of the formation of the desired product B.

The dynamic lag of the ideal separator is negligible when compared to those of the CSTRs, and hence the subsystem equations for the separator are

$$\mathbf{y}_4^1 = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \mathbf{x}_4 \tag{28}$$

$$\mathbf{y}_4^2 = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \mathbf{x}_4 \tag{29}$$

Here, $\mathbf{y}_4^1$ and $\mathbf{y}_4^2$ are, respectively, output stream 1 which contains B and C and output stream 2 which contains A and D. The cost of the separator per unit time is given by

$$f_4 = b(x_{4A} + x_{4B} + x_{4C} + x_{4D})\rho \tag{30}$$

where b is the cost factor of the separator.

With reference to the initially restricted system structure chosen for this example as shown in Figure 2*a*, the imaginary input and output subsystems and their associated objective functions per unit time are

$$\begin{aligned}
&\mathbf{y}_1 = \mathbf{x}_1; \quad f_1 = 0 \\
&\mathbf{y}_N = \mathbf{x}_N; \quad f_N = -\mathbf{v}_N{}^T\mathbf{y}_N \\
&\mathbf{y}_{N+1} = \mathbf{x}_{N+1}; \quad f_{N+1} = -\mathbf{v}_{N+1}{}^T\mathbf{y}_{N+1} \\
&\boldsymbol{\mu}_N{}^T = \mathbf{v}_N{}^T; \quad \boldsymbol{\mu}_{N+1}{}^T = \mathbf{v}_{N+1}{}^T
\end{aligned} \tag{31}$$

where $\mathbf{v}$ is the price vector associated with all the four components in the product stream. The specific process synthesis problem is then to find the system structure parameters as well as the reactor design volumes for the optimal start-up of the given reaction system in the presence of the uncertain reactor temperature variation so as to minimize the overall objective function

$$J = \int_o^{t_f} \sum_{i=1}^{N+1} f_i dt \tag{32}$$

This represents an integral revenue of the desired product B minus the cost of operation and the penalty for the formation of the undesired product C for this time period.

For illustrative purposes, the following numerical values are used throughout the example:

$$\rho = 1.0, \quad t_f = 1.0, \quad K_{10} = 0.5 \times 10^4, \quad K_{20} = 0.8 \times 10^9$$

$$E_1 = 8\,400, \quad E_2 = 20\,000, \quad R = 2.0$$

$$T_i^N = 525^\circ\text{K}, \quad i = 2, 3$$

$$\mathbf{v}_N = (0.0, 3.0, -3.0, 0.0)^T, \quad \mathbf{v}_{N+1} = (0.0, 0.0, 0.0, 0.0)^T$$

$$\mathbf{x}_1(t \leq 0) = (0.0, 0.0, 0.0, 1.0)^T, \quad \mathbf{x}_1(t > 0) = (1.0, 0.0, 0.0, 0.0)^T$$

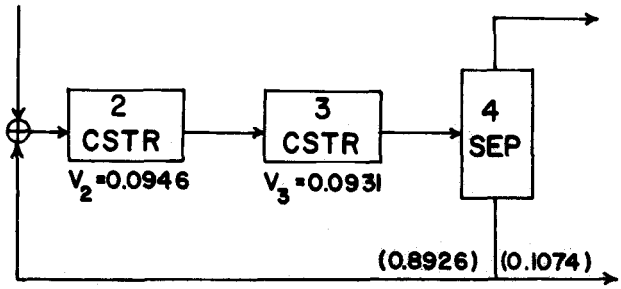
$$\mathbf{y}_i^o = (0.0, 0.0, 0.0, 1.0)^T,$$

$$i = 2, 3 \quad a = 1.0, \quad b = 0.04$$

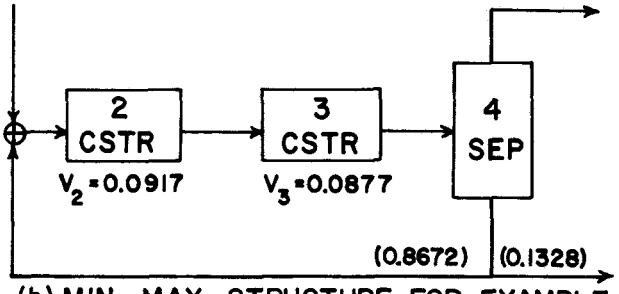
Figure 3*a* illustrates the nominally optimal structure defined by (6) and calculated by the gradient method from the initially restricted system structure shown in Figure 2*a*. The resulting reactor design volumes and the value of the objective function (6) are

$$V_2 = 0.0946, \quad V_3 = 0.0931, \quad \text{and}$$

$$J(\boldsymbol{\alpha}^N, \mathbf{d}^N, \mathbf{q}^N) = -0.01712$$



(a) NOMINALLY OPTIMAL STRUCTURE FOR EXAMPLE 1



(b) MIN-MAX STRUCTURE FOR EXAMPLE 1

Fig. 3. Nominally optimal and minimax structures for example 1.

where the design vector $\mathbf{d}$ represents the volumes of the CSTRs, that is, $\mathbf{d} = (V_2, V_3)^T$, and the time-dependent uncertain parameter vector $\mathbf{q}$ denotes the temperature fluctuations of the CSTRs, namely, $\mathbf{q} = [q_2(t), q_3(t)]^T$. Notice that since the structure parameters α_{22}, α_{23}, and α_{33} in the initially restricted system structure shown in Figure 2*a* are fixed as zero, the preceding theoretical developments suggest that the structure parameter functions should be used within the computational algorithm to check the true optimality of the restricted optimal system structure represented by Figure 3*a* according to (22) and (23). The computed values of the structure parameter functions are

$$M_{21} = 0.172, \quad M_{22} = 0.254, \quad M_{23} = 0.282, \quad M_{24}{}^2 = 0.000$$

$$M_{31} = 0.151, \quad M_{32} = 0.267, \quad M_{33} = 0.348, \quad M_{34}{}^2 = 0.044$$

$$M_{41} = 0.114, \quad M_{42} = 0.210, \quad M_{43} = 0.359,$$

$$M^2{}_{(N+1)4} = 0.000$$

Consequently, the inequality $M_{32} > M_{22}$ indicates that a recycle of a portion of the product stream from the CSTR-2 into its inlet should not improve the system performance. From the results $M_{43} > M_{23}$ and $M_{43} > M_{33}$, the recycles of a portion of the product stream from the CSTR-3 into the inlets of the CSTR-2 and the CSTR-3, respectively, should also not give any better system performance. Hence, the nominally optimal structure shown in Figure 3*a* is truly optimal, even when no restrictions are included in the initially restricted system structure of Figure 2*a*.

By assuming that the reactor temperature fluctuations $q_2(t)$ and $q_3(t)$ are bounded according to (9), with

$$q_i{}^L = -5.0°\text{K}, \quad q_i{}^U = 5.0°\text{K}, \quad i = 2, 3$$

the computed nominal performance index with worst uncertain temperature fluctuations, (7), is

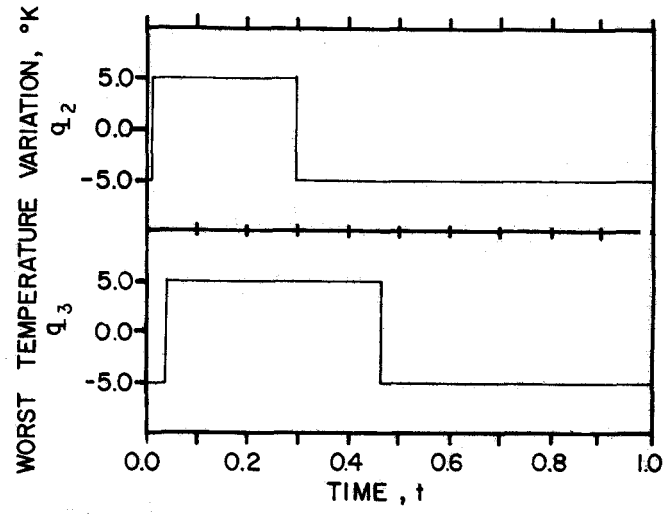


Fig. 4. Worst temperature variations in the CSTRs in the nominally optimal structure in example 1.

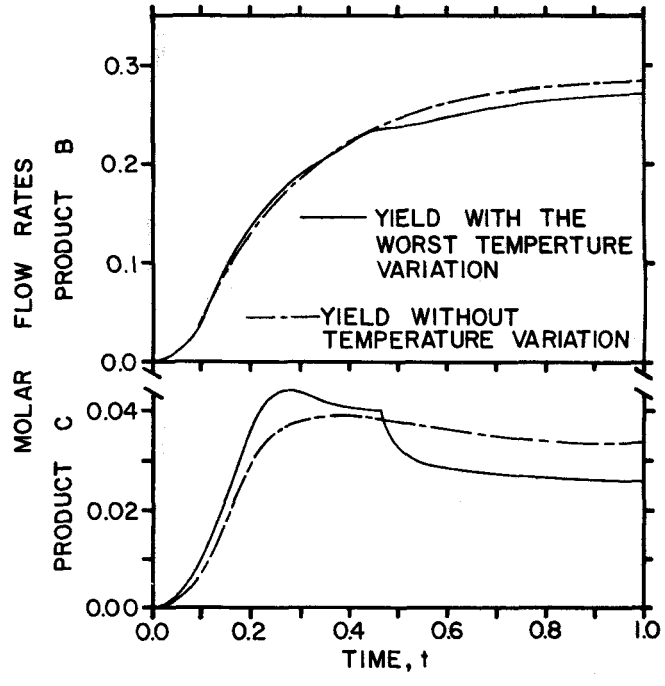


Fig. 5. Optimal profiles of product molar flow rates in the nominally optimal structures with and without the worst temperature variations in the CSTRs in example 1.

$$J(\alpha^N, \mathbf{d}^N, \mathbf{q}^*) = -0.1562$$

Figure 4 shows the corresponding worst temperature fluctuations $q_2(t)$ and $q_3(t)$. The bang-bang characteristics of these temperature fluctuations suggests that the uncertain parameters in this worst-case synthesis tend to increase the Hamiltonians $\overline{H}_i{}^N$ and $\overline{S}_i{}^N$ given by (14) and (15) to their maximum values by staying on the boundary of the admissible uncertain parameter regions $q_i{}^L$ or $q_i{}^U$. The intermediate switching of these uncertain temperature fluctuations between $q_i{}^L$ and $q_i{}^U$ shown in Figure 4 is an indication of the relative importance of the integral revenue of the desired product B vs. the cost of operation and the penalty for the formation of the undesired product C within the start-up period $[0, t_f]$. This is further illustrated in Figure 5, where the changes in the product molar flow rates with time with and without the uncertain temperature fluctuations are compared. For example, the solid curve in Figure 5 shows that the undesirable product C

is formed significantly during the period of $0.04 < t < 0.465$. This formation of the product C is caused by the upper value of the temperature fluctuation in the CSTR-3 as can be seen in Figure 4. For $t > 0.465$, the worst temperature fluctuation of the CSTR-3 is seen to be at the lower bound of $q_3(t)$, and a decrease in the desired product is observed. This is also consistent with the relative importance of the effect of temperature change on the assumed reaction rate constants K_2 and K_3, in which the values of the activation energy and the preexponential constants are quite different.

By using the nominally optimal structure of Figure 3*a* as the initially restricted system structure, a minimax system structure is synthesized by the preceding algorithm. This is shown as Figure 3*b*, with a computed performance index as

$$J(\alpha^o, d^o, q^*) = -0.1580$$

The comparison of Figures 3*a* and 3*b* indicates that the volumes of the CSTRs are reduced in the minimax structure as compared with those of the nominally optimal structure, but the stream split ratio $\alpha_{24}{}^2$ changes its value only slightly in both structures. Also, the values of the three system performance functions $J(\alpha^N, d^N, q^N)$, $J(\alpha^N, d^N, q^*)$, and $J(\alpha^o, d^o, q^*)$ are not significantly different. This is mainly because of the fact that for the isothermal reaction considered, the dynamic behavior of the reactor-separator system is not strongly influenced by the fluctuations in the temperatures of the CSTRs. Consequently, for the present dynamic start-up problem, the optimal reactor-separator configuration and reactor design volumes based on the nominal parameters can be used with a reasonable faith even in the presence of the parameter uncertainty. Generalizing the results of this example, it may be suggested that whenever the uncertain parameters have only a moderate influence on the process dynamics, it is sufficient to consider the use of nominally optimal system structure only, but not the minimax system structure. The above discussions, however, do illustrate the essential features of the proposed concept of the optimal synthesis of dynamic process systems with uncertain parameters and an effective algorithm for providing the quantitative basis for choosing the nominal and minimax system structures. Finally, it should be mentioned that the computation time for using the gradient method in solving this example has been moderate and reasonable. For instance, a CPU time of only about 10 min on an IBM 370/155 computer is needed to obtain the minimax system structure. Judging from the inherent singular bang-bang characteristics of the minimax solution as represented by (17) to (20), it may appear that other computational algorithms developed for the minimax control problems as reviewed and presented by Muralidharan and Ho (1975) may require less computation time. The computational experience in solving the singular bang-bang control problem by the authors, however, seems to suggest that a recently developed algorithm based on the piecewise maximization of the Hamiltonian (Nishida, Liu, Lapidus, and Hiratsuka, 1976*a*, 1976*b*) is most suitable for application to this dynamic process synthesis problem.

In the next example, the effect of uncertain fluctuations in the reactor inlet molar flow rates of reactants on the dynamic start-up of an autocatalytic reaction system will be presented. Here, the uncertain parameters strongly affect the process dynamics, which leads to some minimax system structures that are quite different from the nominally optimal system structures. The important problem of applying proper reactor temperature control to reduce the effect of parameter uncertainty in this dynamic process synthesis problem will also be discussed.

Example 2

Consider a reversible autocatalytic reaction

$$A + B \underset{K_2}{\overset{K_1}{\rightleftharpoons}} B + B$$

where the forward reaction is second order and the reverse reaction is first order. The start-up operation is carried out in a similar manner as example 1, except that the available processing units are only one CSTR and one SEP, and initially the inert material C is present in the CSTR. With reference to the initially restricted system structure shown in Figure 2*b*, the dynamic equations of the CSTR in terms of the molar flow rates of the components are

$$\begin{aligned}
\dot{y}_{2A} &= \frac{1}{\theta_2}(x_{1A} - y_{2A}) - K_1 \frac{y_{2A}y_{2B}}{(y_{2A} + y_{2B} + y_{2C})\rho} + K_2 y_{2B} \\
\dot{y}_{2B} &= \frac{1}{\theta_2}(x_{2B} - y_{2B}) + K_1 \frac{y_{2A}y_{2B}}{(y_{2A} + y_{2B} + y_{2C})\rho} - K_2 y_{2B} \\
\dot{y}_{2C} &= \frac{1}{\theta_2}(x_{2C} - y_{2C})
\end{aligned} \tag{33}$$

where

$$\theta_2 = V_2/(x_{2A} + x_{2B} + x_{2C})\rho$$

is the mean holding time of the reactor, and the other symbols in (33) have the same interpretations as those in (24).

Since the rate of reaction is significantly influenced by both reactants and products, the fluctuations in the inlet molar flow rates of reactants are important uncertain parameter variations. These variations are assumed to be expressed as

$$\begin{aligned}
x_{1A}(t) &= x_{1A}{}^N(t) + q(t) \\
x_{1B}(t) &= x_{1B}{}^N(t) - q(t)
\end{aligned} \qquad t \in [0, t_f] \tag{34}$$

where $x_{1A}{}^N(t)$ and $x_{1B}{}^N(t)$ are the nominal values of the inlet molar flow rates of reactants A and B, respectively, and $q(t)$ is the fluctuation in the flow rate. Furthermore, in the design of a reactor-separator system for the start-up of the temperature-sensitive exothermic, autocatalytic reaction system, great care is required in the proper control of the system. Thus, the temperature $T_2(t)$ of the CSTR is to be manipulated in an optimal fashion so as to give the best performance of the whole processing system subject to the constraint $T_2{}^L \leq T_2(t) \leq T_2{}^U$. The objective function per unit time of the CSTR is assumed to be

$$f_2 = aV_2 + cT_2{}^2 \tag{35}$$

where a is the cost factor for the reactor volume and c is the cost factor for the reactor heating and temperature control. The ideal separator removes only material B completely from the rest of the reaction mixture A and C. Its subsystem equations and objective function per unit time are all similar to (28) to (30). The imaginary input and output subsystems, their objective functions per unit time, and the overall objective function of the whole reactor-separator system are in the forms of (31) and (32). In addition, the following numerical values are used in this example:

$$a = 1.0, \quad b = 0.04, \quad c = 5 \times 10^{-8}, \quad \rho = 1.0$$

$$t_f = 1.0, \quad K_{10} = 0.256 \times 10^5, \quad K_{20} = 0.12 \times 10^9, \quad R = 2.0$$

$$E_1 = 10^4 \quad E_2 = 2 \times 10^4 \quad T_2{}^L = 400°\text{K} \quad T_2{}^U = 600°\text{K}$$

Table 1. Computed Values of Objective Functions in Example 2

	Case 1	Case 2	Case 3
$J(\alpha^N, u^N, q^N)$	−0.13169	−0.27423	−0.41827
$J(\alpha^N, u^N, q^*)$	−0.08610	−0.20452	−0.32416
$J(\alpha^o, u^o, q^*)$	−0.08615	−0.20538	−0.32526
$J(\alpha^o, u^o, q^N)$	−0.13164	−0.27356	−0.41774

$$x_1(t \leq 0) = (0.0, 0.0, 1.0)^T$$

$$x_1(t \geq 0) = (0.70, 0.30, 0.0)^T$$

$$y_1^o = (0.0, 0.0, 1.0)^T, \quad v_{N+1} = (0.0, 0.0, 0.0)^T$$

$$v_N = (0.0, v_{NB}, 0.0)^T$$

where v_{NB} is the sale cost factor of the desired product B to be specified.

Figures 6*a*-1 to 6*a*-3 and Table 1 show the computed results of the nominally optimal structures and the corresponding performance functions, $J(\alpha^N, u^N, q^N)$, for three different values of the sale cost factor of the product B, v_{NB}. The true optimality of these results obtained from the initially restricted system structure has been verified by using the conditions (22) and (23). Figure 6*a*-1 shows that when the cost of separating the reaction mixture is more expensive than the revenue for selling the product B, the output stream from the SEP which includes the unconverted reactant A and the inert material C does not return to the inlet of the CSTR. However, when the costs for separating the reaction mixture and selling the product B are relatively the same, the nominally optimal structure shown in Figure 6*a*-2 includes both recycles from one output stream of the SEP to the inlet of the CSTR and from the output stream of the CSTR to its inlet. Finally, when the cost of product B is more expensive than the previous two cases, the nominally optimal structure does not include a recycle of the product stream of the CSTR to its inlet but has a bypass feed stream to the SEP, as shown in Figure 6*a*-3. This is because when the operating cost of the SEP is relatively low compared with the cost of the product B, it will be economical to send a certain amount of the fresh feed to the SEP and separate the reactant A from the mixture. This then follows by returning the unconverted reactant A to the CSTR rather than feeding all the fresh material to the CSTR. All of these will take advantage of the low separation cost.

In Table 1, the computed objective functions for the nominally optimal structure with the worst uncertain parameter variation, $J(\alpha^N, d^N, q^*)$, show a considerable increase from those without parameter uncertainty, $J(\alpha^N, d^N, q^N)$. In all cases studied, the computed worst variations in the inlet molar flow rates are taken as the upper values of the bounded parameter; that is, $q^*(t) = 0.05$ for $t \in [0, 1]$.

Figures 6*b*-1 to *b*-2 and Table 1 show the computed results of the minimax system structures and the corresponding values of objective functions. The computed worst variations in the inlet molar flow rate are $q^*(t) = 0.05$, $t \in [0, 1]$ for all three cases. The minimax structure for case 1 indicates that the reactor recycle ratio α_{22} increase slightly when compared with that of the nominally optimal structure. For case 2, the minimax structure is somewhat different from the nominally optimal structure, as can be seen from Figures 6*a*-2 and 6*b*-2. Although the nominally optimal structure includes a recycle stream from the SEP to the inlet of the CSTR, this recycle stream is not found in the minimax structure. For case 3, the

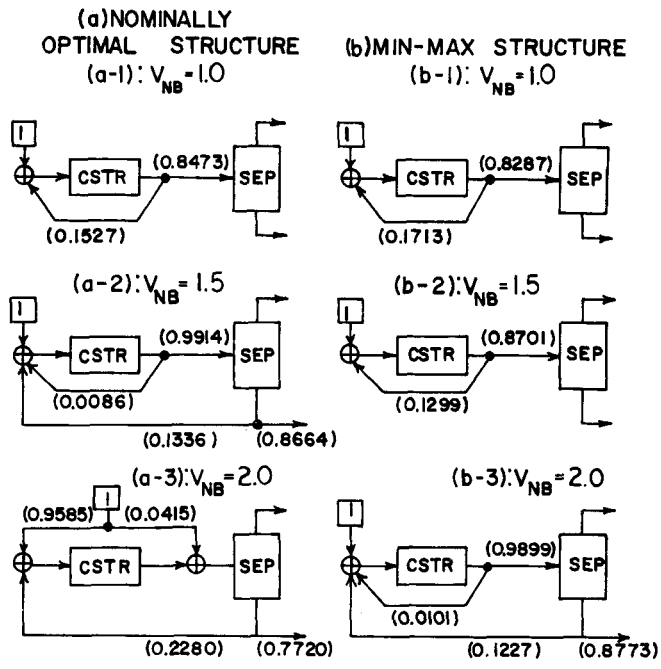


Fig. 6. Nominally optimal and minimax structures for example 2.

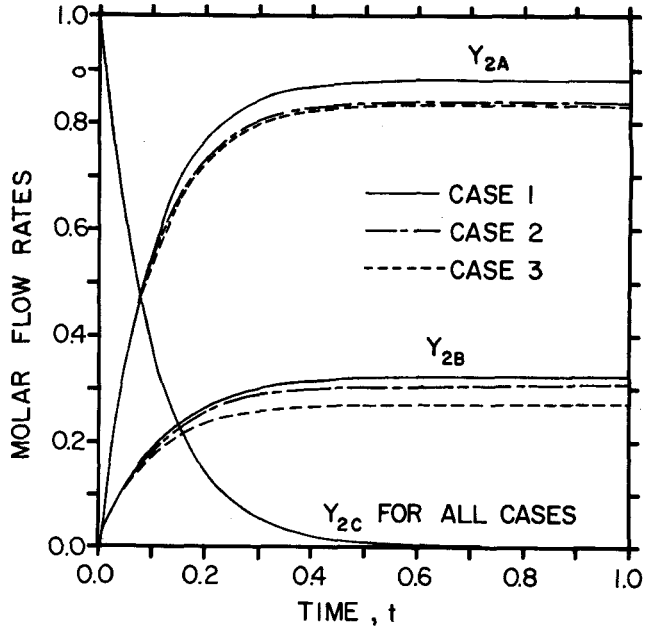


Fig. 7. Optimal profiles of reactant and product molar flow rates in the minimax structure under different cost factors for example 2.

minimax structure is quite different from the nominally optimal structure as seen from Figures 6*a*-3 and 6*b*-3. Figure 7 illustrates the computed molar flow rates for components A, B, and C corresponding to the three cases shown in Figures 6*b*-1 to 6*b*-3. It is seen that with the increase in the cost of the product B from case 1 to case 3, the molar flow rate of y_{2B} is controlled to increase along the entire start-up operation by adjusting the temperature of the CSTR according to the optimal values shown in Figure 8.

The preceding results for this example clearly show that when the uncertain parameters in a given dynamic process synthesis problem have a significant effect on the dynamic behavior of the process, this minimax structure will be generally different from the nominally optimal structure with parameter uncertainty. In this case, the use of the minimax method is recommended, since it gives the process designers an assurance that the actual

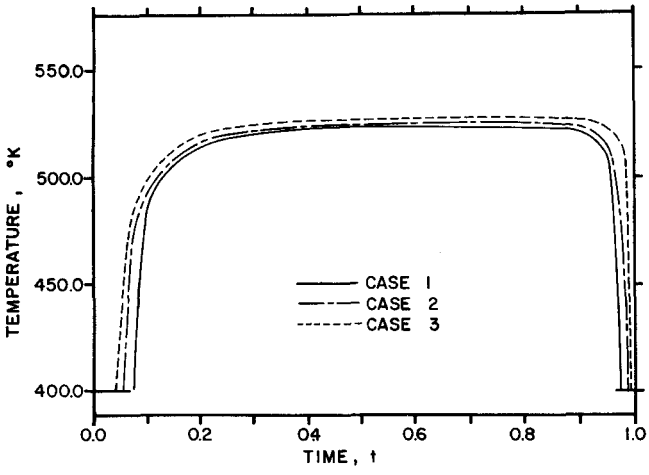


Fig. 8. Optimal reactor temperature control in the minimax structure under different cost factors for example 2.

performance of the process system synthesized will never be worse than that of the minimax structure. Also, the results shown in Figure 6 indicate that the optimal reactor-separator configurations for the controlled start-up of this autocatalytic reaction system are quite sensitive to the changes in the cost of the product B. This suggests that a secondary performance index representing the sensitivity of the original performance index with respect to the cost factor of the product B may be used to form a process synthesis problem with multiple performance measures. Further discussions on this aspect can be found in Liu et al. (1976).

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NOTATION

A = substance A
a = cost factor of reactor
B = substance B
b = cost factor of separator
C = substance C
c = cost factor
D = admissible region of design vector or substance D
$\mathbf{d}$ = design vector
E = activation energy
f = performance function of subsystem
g = right-hand side of subsystem equation
J = performance index of process system
K = reaction rate constant
K_i = set of subsystems incident to y_i
M = number of subsystems or structure parameter functions
P = admissible region of time-independent uncertain parameter
p = time-dependent uncertain parameter
Q = admissible region of time-dependent uncertain parameter
$q(t)$ = time-dependent uncertain parameter
R = ideal gas constant
T = reactor temperature
t_f = final time of process operation
U = admissible region of control vector
$\mathbf{u}$ = control vector
V = volume of reactor
$\mathbf{v}$ = decision variable vector in synthesis defined by $(\alpha, \mathbf{d}, \mathbf{u})^T$
$\mathbf{w}$ = uncertain parameter vector defined by $(\mathbf{p}, \mathbf{q})^T$
$\mathbf{x}$ = input stream state vector
$\mathbf{y}$ = output stream state vector

Greek Letters

α = structure parameters defined by (3) and (4)
ϵ = step size factor
θ = holding time of reactor
λ = adjoint vector defined by (13)
μ = adjoint vector defined by (13)
ρ = molar volume

Superscript

T = transpose
N = nominal value
U = upper value
L = lower value
$*$ = worst value
o = optimal value

Subscript

A, B, C, D = substances A, B, C, and D
(k) = k^{th} trial
i, j, k .. = number of subsystem

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Solution Procedures for Indexed Equation Sets: Structural Considerations

Results are obtained permitting the systematic development of solution procedures for indexed equations by analyzing and combining a number of small problems. The solution procedures obtained are independent of index limits and can be written compactly by using nested FORTRAN DO-loops or equivalent. To illustrate the approach, a solution procedure is developed for a multistage, multicomponent distillation column segment. The solution procedure is valid for any number of stages and components.

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SCOPE

The design or simulation of a chemical process requires finding the solution to a large set of equations (many of them nonlinear). Oftentimes these equations represent either a physical recycling of a process stream from one unit to another or an interaction among variables within a unit; both conditions force a simultaneous solution of the equations. Since the equations are, in general, nonlinear, an iterative solution is necessary. Frequently, convergence of the iterative solution depends on the manner in which the solution is performed. Unless the engineer has special familiarity with the particular set of equations he is trying to solve, he often chooses randomly from among the methods apparent to him. An alternative to this is to develop algorithms suitable for implementation on a digital computer which are capable of analyzing the structural and numerical properties of the set of equations. The computer can then be used to discover how to solve the equations efficiently and dependably. The method chosen to solve a set of equations, whether chosen by the engineer or analytical algorithms, is called a solution procedure.

Two commonly employed types of solution procedures are tearing procedures, such as Gauss-Seidel for linear equations (see, for example, Christensen, 1970), and Newton type of procedures, such as Newton-Raphson (see, for example, Napthali and Sandholm 1971).

This paper deals with the first, tearing. Equations describing real processes are virtually always sparse; that is, although there may exist 1 000 equations in, say, 1 020 variables, each equation will involve only a few variables. It is possible, and one always does it, to take considerable advantage of this structure in developing a solution procedure, often reducing the effort for solving by several orders of magnitude. Tearing procedures attempt to find somewhere near the fewest number of variables possible that one will have to iterate to solve the full set of equations. A 1 020 variable, 1 000 equation example could easily reduce to an iteration involving only thirty variables. To solve, twenty variables would be decision variables whose values we would have to supply externally to reduce the problem to 1 000 equations in 1 000 unknowns. Then, by guessing values for the thirty tear or iteration variables, we can use 970 equations without iteration to calculate values for the other 970 variables in terms of the guessed values for the thirty tear variables. The problem is reduced to one of thirty equations in thirty tear variables, a substantially easier problem.

Newton type of methods for the original problem can take full advantage of the equation structure too by using sparse matrix methods.

All of the algorithms presented in the literature to develop a solution procedure automatically require an explicit representation of each equation and variable before the analysis can begin. For units described by a large number of equations (for example, a fifty plate distillation column with three components can result in 350 equations), application of the above algorithms becomes time consuming and requires large amounts of computer storage space. In chemical engineering design and simulation, the proliferation of equations and variables is quite often due to multicomponent and/or multistage processes, usually modeled with indexed equations and variables. The equations may also arise if one discretizes a differential equation. Great savings of time and computer

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