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Optimal Retrofit Design for Improving Process Flexibility in Linear Systems

by

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ABSTRACT

In this paper the problem of optimally redesigning an existing process to increase its flexibility is addressed A general strategy which first determines the optimal parametric changes and then identifies the optimal structural modifications is presented. For linear models basic analytical properties of flexibility are presented with which very efficient reduced LP and MILP formulations can be developed for parametric and structural modifications. Also, trade-off curves relating flexibility to retrofit cost can easily be generated to provide information on the cost of flexibility. Examples are presented to illustrate the proposed procedures.

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Chemical plants are usually faced with uncertain conditions during their operation. These uncertainties can correspond to variations either in external parameters, such as quality of the feedstreams, product demand, environmental conditions, or to internal process parameters such as transfer coefficients, reaction constants, physical properties. Clearly chemical plants must exhibit good operability characteristics in order to effectively handle these uncertainties.

One of the important components in the operability of chemical plants is flexibility, since it is related to the capability of a process to achieve feasible operation over a given range of the above stated uncertain conditions. Although safety, reliability and dynamic considerations clearly also play an important role, the first important step to enhance the operability characteristics in a plant is to provide for greater flexibility in the operation.

Most of the previous work in process flexibility has concentrated on the problem of designing and synthesizing new chemical plants (Saboo et «/, 1984 [1], Floudas and Grossmann, 1986 [2], Bingzen and Westerberg, 1986 [3], Chen and Prokopakis, 1985 [4]). However, the problem of redesigning systematically an existing process flowsheet to increase its flexibility has not fully been addressed yet (e.g. see Swaney and Grossmann, 1985 [5,6], Linnhoff and Smith, 1985 [7], Kotjabasakis and Linnhof, 1986 [8], Calandranis and Stefanopoulos, [9]). The main difficulty that arises in this problem is the one of how to decide which parameter and/or structural changes are required *\n* the existing process so as to increase its flexibility with the least investment cost. Furthermore, a proper trade-off between flexibility and investment cost must be established.

This paper will present a systematic approach to tackle the problem of optimally redesigning an existing plant in order to increase its flexibility. The main items in the suggested approach *ar*% the following :

- Systematic procedure for handling parametric changes of the design variables.
- Embedding strategy for handling simultaneous structural and parametric changes.

• Procedure for developing trade-off curves between cost and flexibility.

The proposed approach will be restricted to the case when the performance of the chemical plant is described through a linear model. As will be shown in this paper, basic properties of linear models can be effectively exploited so as to perform the above tasks with very efficient LP and MILP formulations.

CONCLUSIONS AND SIGNIFICANCE

In this paper the problem of redesigning the linear model of an existing flowsheet in order to achieve a desired degree of flexibility has been addressed. Taking advantage of some important analytical properties that hold for linear systems, a very efficient MILP formulation has been developed which avoids the need of solving complex embedded optimization problem. Based on this formulation, two algorithmic procedures for determining parametric changes have been presented. As has been shown, these procedures can be extended to handle structural modifications, as well as for generating trade-off curves that provide information on the cost of flexibility and which can help to establish a proper degree of flexibility. Three example problems were presented to illustrate the potential of these formulations.

The significance of this work lies on the fact that it provides a systematic and rational approach to guarantee optimal redesign for improving process flexibility in linear systems.

PROBLEM DEFINITION

The specific problem which is to be addressed in this paper can be stated as follows:

A linear model of an existing flowsheet with fixed equipment sizes and fixed structure is given. Nominal values together with expected deviations are also given for a set of uncertain parameters. The problem is then to determine minimum cost modifications for redesigning the flowsheet so as to increase its flexibility index

In this work the flexibility index as proposed by Swaney and Grossmann [S] will be adopted as the quantitative measure for flexibility. This index provides a measure of the feasible region of operation. Specifically, an index value F-M impliee that a design can handle the specified expected deviations in the uncertain parameters; a value F-1 represents the maximum fractional deviation of expected parameter deviations. This index accounts for the fact that the process can be adjusted during operation through control variables.

It will be assumed in this paper that for the retrofit design the value of the index of flexibility F can be specified as a fixed value (typically F»1), or more generally that it must be determined by establishing a trade-off between cost and flexibility. The case when revenue considerations are also taken into account will be reported in a future paper [10].

As stated above, the performance specifications of a chemical process for feasible operation ere assumed to be described by a linear model. This model will in general consist of a set of equations and inequalities (see Appendix A). For convenience in the presentation, however, it is assumed that the equations are eliminated so as to lead to a set of reduced *linesr* inequality constraints of the following form :

$$fid.z.0) \gg \mathbf{b}_{j}^{\mathsf{T}} \mathbf{z} + \mathbf{b}_{j}^{\bullet} \leq 0 \qquad j \in \mathbf{J}$$

The vector of design variables d defines the equipment sizes. The vector z of control variables stands for the degrees of freedom that are available during operation, and which can be adjusted for different realizations of the uncertain parameters. 0 is the vector of uncertain parameters with nominal value 0^* and expected deviations $A0^*$. Ad' in the positive and negative directions. The region of guaranteed feasible operation of the uncertain parameters will then be defined in terms of the flexibility index F by :

where, for convenience. 0'' is assumed to be a feasible operating point in the existing design. The case when 8^* is an infeasible operating point requires a slight modification of the procedure presented in this paper and is discussed in Pistikopoulos and Grossmann [11].

The following general strategy is proposed to improve the flexibility of an existing flowsheet that is represented by a linear model with uncertain parameters:

- 1. Set a value for the flexibility target F^{v} (e.g. F'*1)
- 2. Evaluate the flexibility of the existing design. If the flexibility index F is greater or equal than F\ stop. Otherwise go to step 3.
- 3. Determine whether *only* changes in equipment sizes is all that is required to meet the flexibility target. If yes. determine the optimal parametric modifications and stop. Otherwise go to step 4.
- 4. Determine the optimal structural and parametric modification to meet the flexibility target.
- 5. Determine the trade-off curve of retrofit cost versus flexibility target. If a new flexibility target is selected go to step 3.

Note that the basic idea in this strategy is to decompose the problem by trying to determine first in step 3 parametric changes if they can be found. In the case when this is not possible, the strategy will try to identify required structural changes in step 4. The strategy as stated cannot necessarily guarantee the global optimum solution. However, as will be shown in this paper, it provides a framework for a better understanding the role of parametric and structural changes. Furthermore, it will be shown that by exploiting the linearity of the model very effective methods can be developed, with which in fact it is possible to consider simultaneous parametric and structural changes.

FORMULATION FOR PARAMETRIC CHANGES

For a given flexibility target F^t, the question that arises in the third step of the proposed strategy is the following: *which* are the *optimal modifications to equipment sizes* for the given flowsheet structure in order to achieve a *desired degree of flexibility*? Or in other words, which are the optimal parametric changes of the design variables? The problem posed in this question can be represented conceptually in the following way:

$$\begin{array}{c} \min \left[\text{Investment cost for changes} \right] \\ \text{s.t.} \qquad F \geq F^{t} \end{array}$$

$$(1)$$

where

- Δd : vector of changes in the design variables d.
- *investment cost for changes* : involves a cost model related to the changes of the design variables Δd .
- F^t: represents the prespecified target for flexibility; it usually equals to one to ensure that the design will meet the expected deviations.

The above problem may have no feasible solution because the only way to attain the desired flexibility target might be through structural changes. In this case one can formulate the problem of determining the largest flexibility that the particular process flowsheet structure can have; that is

> F^{MAX}= max F Δd

It should be noted that F^{1} can be regarded as a *structural flexibility index*, in the sense that according to (2) it indicates the maximum flexibility index that a given flowsheet structure can have when only changes in sizes of equipment are considered.

In order to develop a specific mathematical formulation, assume that fixed charge cost models are used for the investment cost. Problem (1) can then be formulated as:

•

min
$$c^T w \bullet B^T A d$$

w.Ad
s.t. F a F¹ (3)
HJ.'w, £ Ad_t £ U.V, w.«0,1, i«1,r

where the flexibility index F is determined from the MILP problem (see Grossmann and Floudas, 1986 [12]h

$$F = \min_{\substack{j \in J}} i$$

$$g.z.i.s.. j.v.$$
s.t. $s_{i} \cdot f_{i}(d.z.0) \neq 0$ $j \in J$

$$\sum_{j \in J} \lambda_{i} \cdot 1$$

$$\sum_{j \in J} \partial f = 0$$

$$\lambda_{j} - y_{j} \leq 0$$

$$j \in J$$

$$j \in J$$

$$\sum_{j \in J} y_{j} = n_{z} + 1$$

$$\delta'' - i A \$ \cdot * 6 = 6 * * i A 6'$$

(4)

 $a \ge 0$; y, * 0.1; X, . S, 2 0 $j \in J$

In (3) the fixed cost charges c are associated with the vector of binary variables w, while *fi* is the variable-size cost coefficient. The vector of changes in the design variables can be set as Ad - Ad* • Ad\ where Ad\ Ad" are the positive and negative changes of d respectively. These changes are bounded by U", U\ i*1,.,r. where r is the number of design variables.

In (4), S represents the fractional deviation of the parameters, s_j are slack variables, X. are lagrange multipliers associated with the adjustment of control variables z to minimize constraint violations; y_j are binary variables that determine the n+1 active constraints that limit flexibility, where n is the dimensionality of the vector z (see [12] for details)

Problem (3) is clearly a very difficult mixed-integer embedded optimization problem since it has as a constraint problem (4). As will be shown in the next sections, however, problem (3) can be greatly simplified by replacing problem (4) with a set of linear constraints. Since the basic treatment of problems (1) and (2) are similar, only the detailed analysis of (1) will be presented. The final result for (2) will be stated later in the paper.

ACTIVE SETS

The mathematical formulation in (4) involves through the binary variables y_J the selection of the particular set of n*1 active constraints that limits flexibility in the design (see Appendix A for treatment of equations). In order to eliminate the explicit use of the binary variables y_j assume that all the candidate sets of n*1 active constraints in (4) are identified a priori (see Appendix B). The index set for each of these active sets of constaints will be denoted by J_A^{fc} , k-U.n^.

Since a given candidate set of active constraints J_A^k implies a particular selection of the binary variables y_1 problem (4) reduces for each active set k as:

$$S^{k} * \min_{i.i.6} i$$

s.t. Md.z.0) • 0 j 6 J/ (5)

where S^k can be regarded as the '"flexibility index" associated to the set J_A^* ; i.e. it is the maximum fractional deviation of the parameter for the constraints in that active set.

Since the solution i^{k} in (5) must satisfy the constraint 3^{k} S F\ to satisfy F 2 F^f in problem (3), the following equivalent problem can be considered:

where 6^k is given by problem (5). Although the binary variables y_j of problem (4) have been eliminated in formulation (6), the problem still represents an embedded optimization problem; i.e. it has as constraints problem (5) for each active set k.

In the following sections, however, it will be shown that problem (6) can be written explicitly as single optimization problem by representing (5) through a single linear equation.

PROPERTIES FOR LINEAR CONSTRAINTS

In this section it will be shown that 6^k as given in problem (5), can be expessed as a single linear equation in terms of Ad. In order to show this result it will be convenient to reformulate (5) as the equivalent problem [5]:

s.t.
$$f^{k}(6.d) = 0$$
 (7)
6" - i £kd' * 6 £ d" • i A0*

where $f^{k}(6,6)$. the feasibility of design d at the parameter value 6 is given by:

Qualitatively, (7) determines the shortest distance to the boundary of the feasible region $f^*(d,0)$ »O, where *fHd.S*) as given by (8) represents the adjustments of control variables z to minimize the maximum violation of the constraints.

For a given active set J_A^{fe} the function *fHd.S*) has three important properties :

PROPERTY 1 : j^{k} is only % function of d and 6, independent of the control variables z, and is given by:

 $\mathbf{y}^{\mathbf{k}}(\mathbf{d},\boldsymbol{\theta}) = \sum_{j \in \mathbf{J}_{\mathbf{A}}} \lambda_{j}^{\mathbf{k}} \mathbf{f}_{j}(\mathbf{d},\mathbf{z},\boldsymbol{\theta})$ (9) where $\sum_{j \in \mathbf{J}_{\mathbf{A}}} V_{j}^{\mathbf{k}} \cdot 1$. $\sum_{j \in \mathbf{J}_{\mathbf{A}}} X_{j}^{\mathbf{k}} \stackrel{\partial}{\rightarrow} \mathbf{f}_{\mathbf{1}} \cdot \mathbf{0}$

Provided that each nxn square submatrix of the partial derivatives of the constraints f₁, j6J_A^k with respect to the control z is of rank n, then the Kuhn-Tucker

conditions of (8) yield the square system of equations :

$$\sum_{j \in J_A^{k}} \lambda_j^{k} = 1$$
 (10.a)

$$\sum_{j \in J_A^{+}} \lambda_j^{+} \frac{\partial f_j}{\partial z} = 0$$
 (IO.b)

The above system of equations is a linear system because for the linear case \overline{A}_{i} is constant. Also, from the above assumptions (10) is a non-singular square system of (n*1) equations involving (n*i) unknowns in the lagrange multipliers X * (X i* £ 0). Hence, the X* are *uniquely* defined for each active set, and furthermore, they are independent of d and 9.

Furthermore, consider the Lagrangian of the function f*<d,0) in (8h

$$L^{k}(u,z,X) \ll u^{*} \stackrel{\bullet}{\underset{j \in J_{A}}{21}} V < V^{d\#z\#tf} \stackrel{m \ \ u^{k}}{\underset{j \in J_{A}}{11}}$$
(11)

Under the assumption of convexity, at the optimal solution (Bazaraa and Shetty, 1979, [13])

$$f^{*}(d,0) \bullet C (u \ge X^{\#})$$
 (12)

Substituting (10.a) and (11) into (12) leads to:

$$\psi^{k}(\mathbf{d},\boldsymbol{\theta}) = \sum_{j \in \mathbf{J}_{\mathbf{a}}^{k}} \lambda_{j}^{k} f_{j}(\mathbf{d}, \mathbf{z}, \boldsymbol{\theta}_{>})$$
(13)

which then proves the statement in property 1. Also note that from (IO.b) it follows that -5 *0; •••• f^{9} is independent of z.

PROPERTY 2 : For a given active set J_A^k the critical direction for the parameter deviations $A0^{efc}$ is independent of the design variables d.

The critical direction for the parameter deviations, A0^{**k}, must satisfy the inequality $(\overset{\bullet}{[*,-]})^T$ Ad^{ck} > 0; i.e. it is the direction along which there is an increase in the function f^k {4.0).

Consider from (13) the partial derivatives of the function f^{k} in 6 :

$$\frac{\partial \mathbf{y}^{k}}{30} = \sum_{\mathbf{j} \in J_{A}^{k}} \mathbf{x}_{\mathbf{i}}^{*} \frac{\partial \mathbf{f}}{\mathbf{30}}$$
(14)

If we take into account that for the linear case 4 is constant, and that the **30**

multipliers X^{k} are independent of d and 8. then the partial derivative of f^{k} with respect to 8 is clearly invariant to the design variables cL. This partial derivative can be used then to predict *a priori* the critical parameter deviation for the given active set k.

For the case of independent uncertain parameters, the critical direction $A0^{c}_{,}-\$ i=1,..,p can then simply be obtained as follows :

In this way every parameter $8_{\%}$ associated with an active set k can be expressed in terms of 6 and the critical direction as:

PROPERTY 3 : The flexibility index i^k of a given active set J_A^k varies l/nearly with the changes of the design variables Ld.

By making use of (13) and (16), problem (7) can be written as :

$$J^{*} \bullet \min_{\substack{i \\ 1.6.8}} i$$
s.t. $f^{*i6.8} \bullet 21 \qquad \stackrel{\times}{}_{i} * \leq d.z.0) \bullet 0$

$$j \in J_{A}^{*} \qquad (17)$$

where the λ_i^{k} are obtained from (10).

Note that in (17) the dependence of z has been eliminated due to property 1. It is also interesting to see that (17) involves *only* equalities and that the degrees of freedom are given by dim{d}. The latter follows from the fact that there are 1 + dim{ θ } equations, and that δ , d, θ are the variables. This would suggest that for a given value of δ_{σ}^{k} , say at d=d^E, δ^{k} can be expressed as a linear function of Δd through the Lagrangian of (17).

First note that by using (13) δ_{a}^{*} can be determined from the linear equation:

$$\mathbf{y}^{\mathbf{k}}(\mathbf{d}^{\mathbf{E}},\boldsymbol{\theta}_{i}^{\mathbf{N}}+\boldsymbol{\delta}_{i}^{\mathbf{k}}\Delta\boldsymbol{\theta}_{i}^{\mathbf{c},\mathbf{k}})=0 \tag{18}$$

As for the Lagrangian of (17), it is given by:

$$L^{k} = \delta + \nu^{k} \left[\sum_{j \in J_{A}^{k}} \lambda_{j}^{k} f_{j}(d,z,\theta) \right] + \sum_{i=1,p} \mu_{i} \left[\theta_{i} - \theta_{i}^{N} - \delta \Delta \theta_{i}^{c,k} \right]$$
(19)

The stationary conditions of this Lagrangian are :

$$\frac{\partial L^{k}}{\partial \delta} = 1 - \sum_{i=1,p} \mu_{i} \left[\Delta \theta_{i}^{e,k} \right] = 0$$
(20)

$$\frac{\partial L^{k}}{\partial \theta_{i}} = \mu^{k} \sum_{j \in J_{k}} \lambda_{j}^{k} \frac{\partial f_{j}}{\partial \theta_{i}} + \mu_{i} = 0 \qquad i=1,..,p \qquad (21)$$

Multiplying equation (21) by $\Delta \theta_i^{*,*}$, adding over i and combining it with equation (20), the following expression can be obtained for the multiplier r^* :

$$\nu^{k} = -\{\sum_{i=1,p} \Delta \theta_{i}^{ak} \sum_{j \in J_{A}^{k}} \lambda_{j}^{k} \frac{\partial f_{j}}{\partial \theta_{i}}\}^{-1} \quad k=1,..n_{AS}$$
(22)

With this multiplier, one can calculate the sensitivity coefficients σ_i^k , defined as the partial derivatives of the flexibility index δ^k with respect to the i'th component of the vector d of the design variables; namely :

x

Since from (17) the multiplier r*»- -3-5-. it follows from (13) and (23) that

$$\sigma_{i}^{k} = -\nu^{k} \sum_{j \in J_{k}} V |^{h} \qquad i * W$$
(24)

Further, since the above sensitivity coefficients are constant, the flexibility index of a given active set k can be written as:

$$i^k \ll i \wedge 2 \wedge M \wedge Ad, \qquad ks1-nA\$$$
 (25)

where 3_o^k is the flexibility index for the existing design d^{*} and can be determined from (18).

This then shows that for a given active set, where the partial derivatives of f_j with respect to z are linearly independent, i^* as given in problem (5) can be expessed by (25) as a linear function of Ad in terms of the sensitivity coefficients a_j in (24). These coefficients can clearly be determined with simple calculations.

It should be noted that wh«n the assumption of linear independence does not hold, the expession in (25) can still be obtained through the direct numerical solution of problem (5), or equivalently from problem (4) at a given active set. Let X_j^* be the multipliers of the equations in problem (5). Then :

$$\sigma_{i}^{k} = \frac{\partial}{\partial d_{i}}^{k} = \sum_{j \in J^{k}} \frac{\partial}{\partial f_{i}}^{j} \frac{\partial}{\partial f_{i}}^{j} \frac{\partial}{\partial d_{i}}^{j} = -\sum_{j \in J^{k}} \overline{\lambda}_{j}^{k} \frac{\partial}{\partial d_{i}}^{j} \frac{f_{i}}{\partial d_{i}}$$
(26)
where $\overline{X}_{ik} = -\frac{\partial \delta^{k}}{\partial f_{i}}$

REDUCED FORMULATIONS

The importance of equation (25) is that problem (6) can be greatly simplified since it can be formulated in terms of the changes of the design variables Ad. and the flexibility index 6^* for each active set k. Specifically, problem (6) reduces to the MILP

$$\min_{w,Ad} c^{T}w \cdot /J^{r}Ad$$
s.t. $6^{*} * F^{f}$

$$k \gg 1,..,n_{r}$$

$$\delta^{*} = \delta^{*}_{q} + \sum_{i=1}^{r} \sigma_{i}^{*} \Delta d_{i}$$

$$(PC)$$

$$- U_{i}^{*} w_{i} \in Ad \in U_{i}^{*} w_{i} = 0, 1, i = 1,..,r$$

$$\delta^{k}ZO. Ad \in \mathbb{R}^{r}$$

By applying a similar procedure to problem (2) for finding the structural flexibility index, it can be shown that it can be reduced to the following LP:

3^0, Ad6FT

Note that both problems are no longer embedded optimization problems, and that the sizes of (PC) and (PF) are small since they involve only one equation for each active set k, and i^{k} and Ad as variables. The next section will show how (PC) and (PF) can be incorporated in algorithmic procedures for determining parametric changes to improve flexibility.

ALGORITHMS FOR PARAMETRIC CHANGES

Based on the properties and the condensed formulations presented in the previous sections, two algorithms can be developed to find the optimal parametric changes or maximum structural flexibility index The first algorithm is suitable for a modest number of active seta and assumes linear independence of the partial derivatives of the constraints $f_{ij} \in J_A^k$ with respect to the control z. The steps in this algorithm are as follows :

ALGORITHM 1

STEP 0 : Specify the flexibility target F* and find tha flexibility index F of the existing flowsheet If F i F\ stop.

STEP 1 : Identify all the n[^] active sets (see Appendix B).

STEP 2 : For each active set $J_A \setminus k-i^n$:

a. Calculate X_{j}^{k} by solving the linear system of equations in (10h define p^{*} as in (13).

b. Obtain the critical vertex direction A0,*-* from tha signs of the gradient of f^{*} with respect to \$ aa In (151

c Calculate the multiplier ** from aquation (22).

d. Calculate tha sensitivity coefficients $\#_{i}^{k}$ from aquation (24).

a. Obtain tha flexibility index $J^*_{\#}$ for the existing design d^8 from the linear aquation in (181

STEP 3 : (a) Solve the MILP problem (PCX

(b) If the MILP solution is feasible, tha new vector of the design variables will be given by

16

• d* • Ad

where d* is the vector of existing design variables.

(c) If the MILP is infeasible the maximum structural flexibility can be determined by solving the LP problem (PF).

An important feature of this algorithmic procedure is that, by taking advantage of the analytical properties that hold for the linear case, it requires just a sequence of simple algebraic calculations and the solution of a reduced MILP *In* step 3. It should be noted that this MILP may be reduced to an LP problem if fixed charge costs are not considered.

The drawbacks of the above procedure lie on the possible combinatorial problem related to the identification of the possible active sets in step 1, and to the assumption of the linear independence in the gradients of the constraints. These limitations can be overcome with a second algorithm in which the MILP for th* flexibility index in (4) is solved succesively to identify only these active sets with J* \pounds F \ and to obtain the values of the multipliers \overline{X} .

ALGORITHM 2

STEP 0 : Specify the flexibility target F^f, set k»1.

STEP 1 : Solve (4) to obtain $i \mid J_A M_i$ If $i^{\%} * F \mid$ stop.

STEP 2 : (a) Set k « k • 1

(b) Add an integer cut to (4) (see Appendix B) to exclude J_A^* and solve the MILP in (4) to obtain J_A^* .

(c) If $S^k \pounds F^*$ go to step 3; otherwise go to 2(a)

STEP 3 : Calculate the sensitivity coefficients $< x_i^k$ from

$$\sigma_{i}^{*} = -\sum_{j \in J_{A}^{*}} T_{j} \partial_{t} f \quad i > 1 r \qquad (2e)$$

STEP 4 : (a) Solve the MILP (PC).

- (b) If feasible solution , set d^* " » d^{\in} Ad, go to step 1.
- (c) If *no* feasible solution, solve problem $F^{1,1}$ in (PF), stop.

It should be noted that in step 2(b) \overline{X}_{μ} is obtained from the dual prices corresponding to the first set of equations in the MILP problem in (4). Furthermore, the set $J_A{}^k$ is defined by the binary variables y_j that take a value of one in (4). It should also be observed that usually there is no need to explore all the possible combinations n_{AS} of the active sets in this algorithm. The reason is that in steps 1 and 2 only the active sets with $\mathscr{E} F^*$ are determined. On the other hand the price one has to pay with this scheme is that additional iterations might be required as indicated by step 4-db) in which the flexibility index must be evaluated for the design modification due to the fact that not all active sets are explicitly considered in (PC).

TRADE-OFF CURVE FOR COST vs. FLEXIBILITY

In the algorithmic procedures described in the previous section, the flexibility target F^1 is specified at a fixed value, usually 1.0, to ensure that the design will meet the expected deviations of the uncertain parameters.

In this section it will be shown that an additional advantage of these algorithms is that they can be easily extended for the construction of a trade-off curve of cost vs. flexibility that provides information on the cost of flexibility. To show how this extension can be performed, assume that the MILP in (PC) reduces to the following LP by eliminating the fixed-cost charges:

$$\min_{\Delta \mathbf{d}} \sum_{i=1}^{r} \boldsymbol{\beta}_{i} \Delta \mathbf{d}_{i}$$

s.t. $\boldsymbol{\delta}_{\bullet}^{\mathbf{k}} \cdot \sum_{i=1}^{r} \boldsymbol{\sigma}_{i}^{\mathbf{k}} \Delta \mathbf{d}_{i} \geq \mathbf{F}^{\mathbf{k}} \qquad \mathbf{k} = \mathbf{1}, \mathbf{n}_{\mathbf{AS}}$ (27)

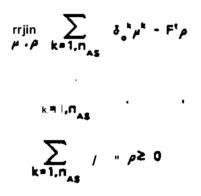
In order to develop a trade-off curve of cost vs. flexibility (27) must be solved parametrically in terms of F\ This might *in* principle require the solution for a very large number of values of F'. However, this can be avoided as follows. Problem (27) can also be rewritten as the following maximization problem :

$$\max_{\Delta d_{i}} -\sum_{i=1}^{r} \beta_{i} \Delta d \qquad (28)$$

S.t. $a = \sum_{i=1}^{r} \sigma_{i}^{*} \Delta d \leq \delta_{o}^{*} \qquad k=1...n_{AS}$ (a)
 $- (x = x^{*})^{*/2}$ (b>

where a is a scalar.

If we consider the dual problem of (28), it is of the following form :



where

/i^k vector of multipliers of inequalities (a) in (28)

p the multiplier for the single inequality (b) in (28)

It should be noted that / is the cost of flexibility, because it represents the change of the cost with respect to the change of the flexibility target F\ Also, it should be noted that the trade-off curve relating flexibility to cost will be a piece* wise linear function where each segment is characterized by different limiting active sets identified by the multipliers $?^k$. This would then suggest that for generating the trade-off curve of cost versus flexibility it suffices to identify the break points in the curve.

Based on (29) the procedure to generate the break-points in the trade-off curve is as follows :

1. Pick as a starting point for F^{f} the flexibility index of the existing process.

which corresponds to $F^{t} = \min_{L} \delta_{0}^{k}$

- 2. Solve the dual problem (29) to evaluate the multipliers μ^{t} , which will provide the information of which active sets are the limiting ones, and the value of ρ , which will correspond to the cost of flexibility.
- 3. Do range analysis (see Schrage, 1984, [15]) at the solution of (29) to determine what is the allowable increase δF for F^t such that the multipliers μ^k will remain unchanged (i.e. same limiting active sets and therefore constant value for ρ).
- 4. Set the new break point $F' = (F')_{\alpha \mid n} + \delta F$ and go to 2.

From the above it is clear that by solving a sequence of dual problems in (29) coupled with the range analysis, the break points of the different segments in the trade-off curve are identified. Furthermore, each segment has a slope given by ρ , the cost of flexibility. Thus, only a finite number of points will be considered without having to explore the infinite number of values for F^t. Finally, in order to avoid possible problems of degeneracy solving the dual problem (29) in step 2, the value of F^t should be set F^t = F^t + ϵ where ϵ is a small number (e.g. ϵ = .001).

For the case when fixed-cost charges are included in the MILP problem (PC), a similar but somewhat more involved procedure is required to generate the trade-off curve as shown in Appendix C.

EXAMPLES

Two examples will be considered to illustrate the application of the proposed algorithmic procedures for parametric changes.

The first one will be small linear example, which will serve as an illustration of the procedure of algorithm 1. Additionally, the trade-off curve relating flexibility to cost will be constructed to illustrate the procedure described in the previous section. Example 2 will correspond to the linearized model of a flowsheet problem, where due to the large number of possible active sets, algorithm 2 will be applied. EXAMPLE 1

Consider that the specifications of a design are represented by the following inequalities :

 $f_{f} * z - 9 \cdot d_{t} - 3 d_{2} \pounds 0$ $f_{2} = -z - \frac{9}{3} \cdot d_{2} + \frac{1}{3} \pounds 0$ $f_{1} = z \cdot \theta - d_{1} - 1 \le 0$ (30)

These inequalities involve a single control variable *i.* two design variables d_{t} , d_{2} and a single uncertain parameter 9 specified within the range 0£ 9 £ 4.

Its existing design is $d_t^{f} * 3$ and $d_2^{\$} \cdot 1$. By examining the plot of the function f(6,z.d) for the existing design in Fig. 1 (ii), it is clear that for $0 \pounds 8 \pounds 1$ there is infeasible operation, whereas for $1 \pounds 9 \pounds 4$ there is feasible operation. Then the question to be answered is what are the appropriate changes of the design variables d_i and d_2 in order that the new design be feasible for the whole operating range of the uncertain parameters 8.

Applying the procedure of algorithm 1, the following results are obtained:

Step 1 : Since n*1«2. two active sets can be identified from the following two equations in (10) : (i) $X_f \cdot X_2 \cdot X_3 \cdot 1$ and (ii) $X_1 \cdot X_2 \cdot X_3 \cdot 0$. The first active set J_A^{\dagger} involves f_f and f^{\uparrow} and the second one J_A^{\dagger} . involves f_2 and $f_{\%}$.

Step 2 (i) : Por active set $J_AM1.2$) the multipliers X^X ,¹ calculated from (10) yield $X_1^{1} \ll X_2^{1*}.S$. Since from (13) the function $f^1 \ll 2[1-tf]/3$, the critical direction corresponds to the lower bound 0° «O. The value of v¹ calculated from (22) is $*^1 \ll ...75$. With this, from (24) the sensitivity coefficients $< r^{*}...27S$, $< r_2^{1*}...75$ w% obtained. Finally, the value of a^'O.S from (18K

Step 2 tii) : For active set J_AMZ3 the multipliers X_2^2, X_3^2 calculated from (10) yield $X_2^2=X_3^{2*}.5$. Since from (13) p'*[0-4]/3, the critical direction corresponds to the upper bound $0^{c,2*}4$. The value of r² calculated from (22) is *^{2*}-1.5. With this, from (24) the values of the sensitivity coefficients * ** *^{3*}_3-.75 are obtained. Finally, the

value of 5^{2*1}_{2*1} from (18).

Step 3 : Assuming cost coefficients c^c^O, $fl_x^m fl_2^{m<} W^*$ problem (PC) can be formulated as the following LP :

The solution to the above LP is $Ad^Ad_2 * 1.335$. This means that in order to achieve flexibility greater or equal to one (i.e. feasible operation for the whole operating range $OS8\pounds 4$) at minimum cost, both design variables should be increased by 1.335 taking the values :

The effect of the redesign over the existing system can be seen in Figure 1. Figure I.iii shows the feasible region of the redesigned model and in Figure Liv its corresponding function f is plotted, whereas Figures I.i and 1.ii show the feasible region and the function f for the existing design.

It should be noted that the most economical feasible redesign corresponds to the one where both the design variables should change in such a way that the flexibility index for both the active sets will be equal to one.

It should also be noted that if problem (PF) is solved, the flexibility index F is again equal to 1 (i.e. $F^{mmm} \cdot 1$), but a different redesign is obtained with [d_i'*^w«i2, d₂^{NCW}«6.16]. Figure 2 shows its feasible region. The above result clearly indicates that there are usually alternative values of the parametric design variables to achieve a flexibility index F \cdot 1.

Finally, to illustrate the development of the trade-off curve, the LP in (31) is rewritten as :

$$\begin{array}{rll} \text{max} & \text{MOAd,} & - & \text{IOAd}^{\wedge} \\ \text{s.t.} & .375\text{Ad}_1 & - & .75\text{Ad}_2 & \bullet & \texttt{a} \ \pounds \ 0.5 & & & (32) \\ & & - & .75\text{Ad}_f & \bullet & .75\text{Ad}_2 & \bullet & & \texttt{e} \ 1 \\ & & & - & * \ S & - \ F^1 \end{array}$$

Its corresponding dual will be :

Applying the procedure for constructing the cost curve, the following results are obtained :

- For FM).501 (current flexibility index) (33) yields /#,*13.33 and ^0 and a value of 13.33 for the cost of flexibility *p*. which remains constant doing the range analysis up to F^{**}0.75. This indicates that for the range of 0.5 \pounds F¹ \pounds 0.75 only active set (1) is the limiting one and the corresponding segment for this range starts from (0.5,0.0) and ends at (0.75,3.33) at the cost vs. flexibility curve.
- Setting $(F^{*}O^{SI}, active sets (1) and (2)$ become both limiting with $/i, {}^{s}56, {}_{,2}*27.33$ and the value of the cost of flexibility *p* yields 93.33. This indicates that for the range $F^{*}
 e 0.75$ the slope of the second segment is significally increased, due to the fact that both design variables d, and d₂ must be changed, whereas for the first segment only a change in d, is required. The second segment starts from (0.75,3.33) and passes through (1, 26.66) at the cost vs. flexibility curve. The resulting trade-off is shown in Figure 3.

EXAMPLE 2

The flowsheet of a chemical process is presented in Figure (4). It involves a PFR reactor, where a reaction of the form A • B takes place and a fractionator (separation column), which separates the final product from the top whereas recycles to the reactor the unreacted A. Two pumps are used; one for the feedstream and one for the recycle stream. The feedstream contains both A and B. Some purging also exists in the recycle stream for control purposes. Sizes and cost data of the existing design are given in Table 1.

Three uncertainties are involved in the description of this system : one in the fraction of B in the feedstream with nominal value of 0.05 and deviations 0.045 in both directions; the remaining two in the reaction rate constants k, and k_2 with nominal values 0.2 s'¹ and 0.1 s"\ respectively, and corresponding deviations 0.05 s^{*1} and 0.02 s'

The linearized model of this process at the nominal operating conditions involves 18 equations and 9 inequalities in 21 unknowns. Elimination of the state variables (see Appendix A) leads to 9 inequality constraints with 3 control variables, the pressure P and the temperature T of the separation column, and the flowrate of the feedstream $F_{,N}^{N}$. Also there are 3 design variables, the volume V of the PFR reactor and the powers W_{t}° and W_{2}° of the two pumps. The flexibility index for the existing design is 0.31. Therefore, a redesign is required to increase the flexibility index to a value of 1.

From Appendix B, it can be determined that the number of possible active sets for this process is 25. However, if one applies the procedure of algorithm 2 only two active sets must be considered. These involve two design variables: the volume V of the reactor and the power W_{3}° of the pump of the recycle stream. Using the cost data in Table 1 the solution obtained is a change only of the volume V from 7.5 to 14.64 m³ with a cost for the modification of \$714,000. Therefore, the flexibility of the linearized model of the process flowsheet in Figure (4) can be increased from 0.31 to 1.0 at minimum cost by adding a reactor in series with a volume of 7.14 m³.

It should be noted that if a nonlinear calculation of the flexibility index is performed for the redesigned process (see Grossmann and Floudas, 1986, [12]) the value obtained is 0.8. This result simply indicates that the linear model has only provided an approximate solution to the nonlinear model of the process flowsheet Finally, applying the procedure for constructing the trade-off curve yields the curve shown in Figure 5, which has a cost of flexibility of 10.3x10⁹ \$/F. Note that in this case there are no break-points as there is only one active set defining the curve.

STRUCTURAL MODIFICATIONS

The third step of the proposed strategy deals with the problem of modifying appropriately the flowsheet structure in order to achieve the flexibility target.

For linear models, the above stated problem can be addressed through a direct extension of the mathematical formulation of the MILP in (PC). This extension

involves first the development of a general superstructure for the possible structural modification alternatives. By modelling the superstructure with the MILP in (PC), the resulting optimization problem will tackle both the problems of parametric and/or structural modifications for increasing the flexibility of a given linear process model at a minimum cost.

One of the questions that obviously arises is how such a superstructure can be developed in a systematic way. A possible "building" criterion for the superstructure can be based on the design variables d associated with the critical active set found in problems (PC) or (PF); structural modifications are to be assigned for these design variables that give rise to a nonflexible behaviour.

The following example problem will serve as a motivating illustration of the ideas on structural modifications for linear systems.

EXAMPLE 3

The block diagram of the chemical complex considered in Grossmann, Orabbant and Jain [14] is presented in Figure 6. The economic data for this chemical complex are shown in Table 2, and its six capacity variables for the existing design appear in Table 3. Five uncertain parameters have been considered corresponding to a demand of chemical G in the local market (d_y) , and upper bounds for purchases of chemical A and B and sales of chemical I and G in the international market $(6^{A} B_{\%}, 0_{y} d_{A}$ respectively). The nominal values and the expected deviations of the uncertain parameters are given in Table 4.

This system can be described with thirteen linear inequalities and five control variables, with an upper bound of 1287 possible active sets. For the existing design, the flexibility index is calculated to be F^{w} «0.32, which clearly indicates that redesign is required for the system to handle the expected deviations of the five uncertain parameters.

Algorithm 2 has been applied to this problem. Only four active sets **are** identified by solving successively the MILP in (4) with integer cuts and up to the point

where the active set leads to $S^{k} * 1$. The constraints in the active sets involved only three design variables d_f, d₄, d_f. Applying the MILP in (PC) it was determined that only one change is required, namely the design variable d_§ from its existing value of 40 Kg/hr to 60 Kg/hr with a cost for the modification of \$44.6x10*. Therefore, the flexibility of the chemical complex in Figure 5 can be increased from 0.32 to 1.0 at minimum cost by expanding the capacity in process 6 up to 60 Kg/hr.

Suppose now that the largest increase in capacity that can be achieved by redesigning the existing process 6 is 50 Kg/hr. Then, problem (PC) becomes infeasible for the flexibility target F^{f} »i. Applying problem (PF) the maximum structural flexibility yields a value of 0.67 IP^{**1} • 0.67). Therefore, doing only parametric changes it is impossible to meet the flexibility target of 1.0. and hence some structural modification must be considered. The solution of (PF) provides the information that design variable d_f is the only one associated with the critical active set. Therefore, applying the "building" criterion for the superstructure, a structural modification is to be proposed around process 6 (d_§), which is responsible for the inflexible behaviour of the system.

A new alternative process 6^* . which produces J from I is considered in parallel to the existing process 6. This is a more efficient process than 6 because it requires lower operating cost (\$/Kg) as it appears in Table 2. Applying the MILP in (PC2) the result indicates that the new alternative process 6^A should be selected because it can handle the whole range of expected deviations for the uncertain parameters. The new redesign of the complex exhibits a flexibility index of 1.0 for a capacity of 60 Kg/hr of process 6^A with a cost for the modification of \$150x10*. Therefore the flexibility of the chemical complex can be increased from 0.32 to 1.0 by replacing the existing process 6 with new process 6^* of capacity 60 kg/hr.

This example shows how a superstructure might be derived in order to tackle in an efficient way the problem of simultaneous parametric and/or structural modifications for improving process flexibility.

ACKNOWLEDGEMENT

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APPENDIX A. TREATMENT OF EQUATIONS FOR IDENTIFYING ACTIVE SETS

The physical performance of a chemical process in the steady-state can be described by the following set of constraints

where h is the vector of equations (i.e. mass and energy balances or equilibrium relations) which hold for steady-state operation of the process, and g is the vector of inequalities (i.e. design specifications or physical operating limits) which must be satisfied if operation is to be feasible.

In order to identify the possible active sets in (A1) it is required to eliminate the equalities to obtain the stationary conditions of problem (8). In order to obtain equation (10.b), this elimination can be done as follows :

The stationary conditions of *fid.z.0*) with equalities are of the form (see Grossmann and Floudas (1986)h

From (A2)(i) the multipliers / can be obtained from:

$$/ \cdot - [V^{T} h] " [X^{T} V/g]$$
 (A3)

Substituting (A3) into (A2XH) leads to:

$$[- VJh(V/h) - V/g \cdot V/g] X' - 0'$$
(A4)

which are precisely the stationary conditions in (IO.b).

APPENDIX B. IOENTIFICATIOM OF ACTIVE SETS

All the potential active sets n_{AJ} in problem (4) are given by those combinations of the binary variables $y_{ij} \in J$ which have n+1 non-zero components and satisfy the following equations in problem <4h

$$\sum_{j \in J} \lambda_{j} \frac{\partial f_{j}}{\partial z} = 0$$

$$(BD)$$

$$\sum_{j \in J} y_{j} \cdot n \cdot 1$$

$$\lambda_{j} \ge 0, y_{j} = 0, 1 \quad j \in J$$

To identify the potential active sets it is convenient to define matrix which will have as components the signs of the gradients V_{r} Mid.z.0). That is.

$$\mathbf{a}_{\mu} = \begin{cases} 1 & \frac{\partial f_{\mu}}{\partial z_{\mu}} > 0 \\ -1 & \text{if } -J_{\mu} = \langle 0 \\ z_{\mu} \rangle \end{cases}$$
(B2)
$$0 & \text{if } \mathcal{L}_{-}^{\text{lf}_{p}} = 0 \end{cases}$$

Any active set can be obtained by solving the following MILP :

min
$$0^{\mathsf{T}} \mathsf{y}$$

S.L A $\mathsf{y} \cdot 0$ (B3)
 $\sum_{j \in J} \mathsf{y}_{j} \cdot \mathsf{n} \cdot 1 \mathsf{y}_{i} \cdot 0.1 j \in J$

However, since all the active sets must be identified the following procedure can be used :

- Step 1 : Set k»1.
- Step 2 : Solve the MILP in (B3) to obtain the solution y^k . If there is a feasible solution define the active set $J_A^{k*}{j/y_i^*}^S U$. If there is no feasible solution, stop.
- Step 3 : Add to the MILP the integer cut

$$\sum_{j \in J_A^{k}} y_j^{k} \sum_{j \notin J_A^{k}} y_j^{k} \leq n$$

to exclude the active set $J_A{}^k$ for the next solution. Set k=k+1, return to step 1.

It should be noted that for problems of small size the list of active sets can simply be obtained by exhaustive enumeration. APPENDIX C. TRADE-OFF CURVE FOR COST vs. FLEXIBILITY - MILP case

In this Appendix^{*} it will be shown how the trade-off curve of cost vs. flexibility can be obtained when fixed cost charges are included in (PC). A typical trade-off curve for this MILP problem is shown in Figure C1. It exhibits two important features : (a) it is discontinuous at the break points defined by the change of the limiting active sets; (b) it might be piecewise continuous within the region characterized by the same limiting active sets due to a change of the design variables to be modified.

The above features suggest that for generating the MILP trade-off curve it suffices to identify the points of discontinuity (i.e. change of the limiting active sets), as well as the possible break points within the region associated to a given active set. This set of points will be denoted by F¹ with cost z^1 , $j^* 1,2$ The following procedure is proposed :

1. Set /*\ j-1. F'-F¹.

2. Solve MILP problem (PC) to identify its corresponding active sets J^{ℓ} , and the nonzero changes of the design variables Ad, i \in where J^{A} kl J_{A}^{k} limiting active set}, and I^{J*} {il w,*1). Set optimal objective function value to z^{j} .

3. For the nonzero changes of design variables I^* apply the procedure for the LP case to identify the allowable increase 3F' for F^J. This corresponds to doing range analysis at the solution of the dual of the following problem (CD :

$$\min_{\Delta d_i} \sum_{i \in I^j} \beta_i \Delta d_i$$

s.t. $\delta_{\bullet}^{i t} + \sum_{i \in I^j} \sigma_i^{i t} \Delta d_i \ge F^j$ $k=1, n_{AB}$ (C1)

4» In order to determine the increase JF" that is due to a change in other design variables for the same active set in Jr solve the following MILP problem :

- U," w, £ Ad ≤ U,^{*} _{Wt} .<mark>w,</mark>=0,1 ,i=1,.,r

5. (a) If 5F"< 5F-, set F'*'»F^J*3F". z'^z". l^j*'«{il w «1), j«j*i. go to step 3.
(b) If iF"*3F\ set P"'P*iFX'I*\ j»j*i. go to step 2

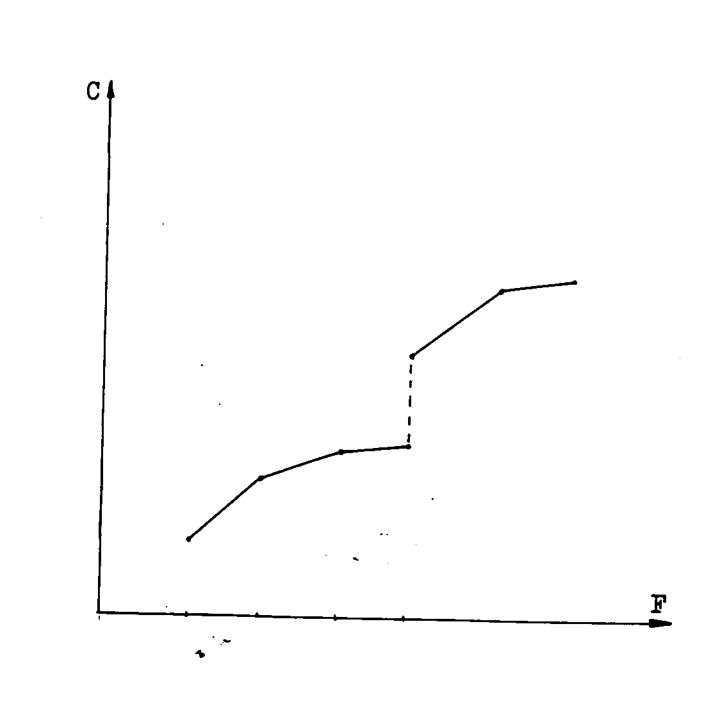


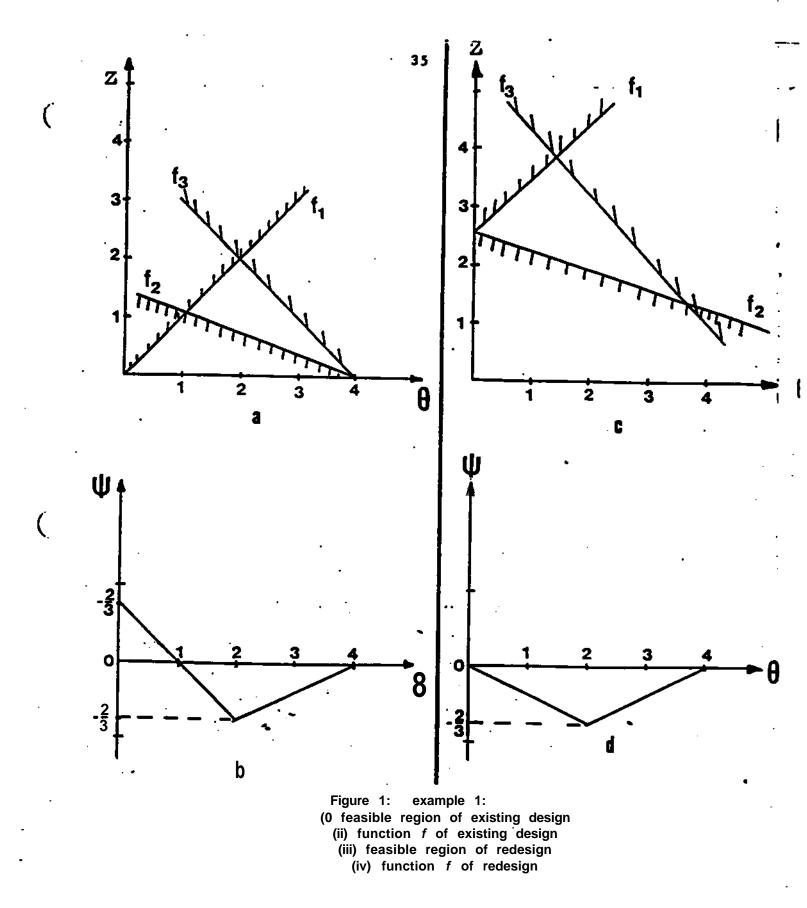
Figure C-1: Typical trade-off curve-MUJ> case

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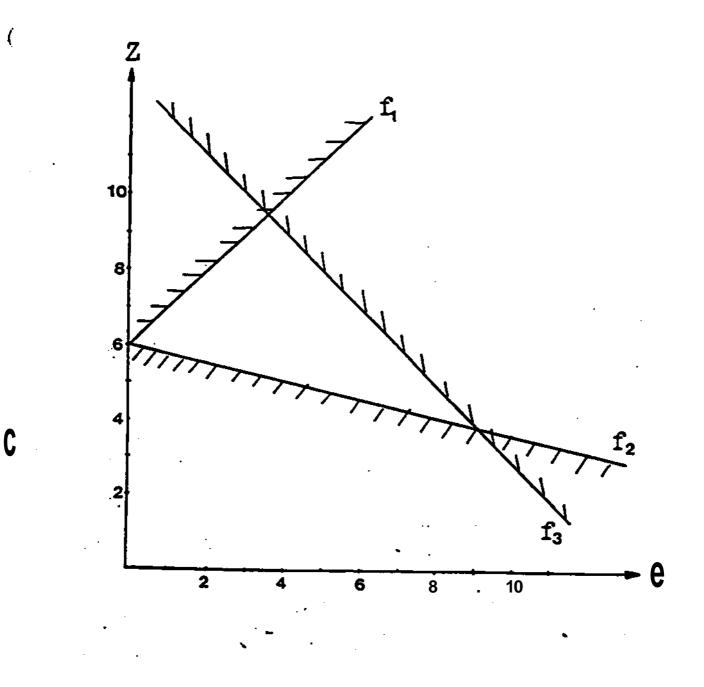


Figure 2: Feasible region of max f problem for example 1

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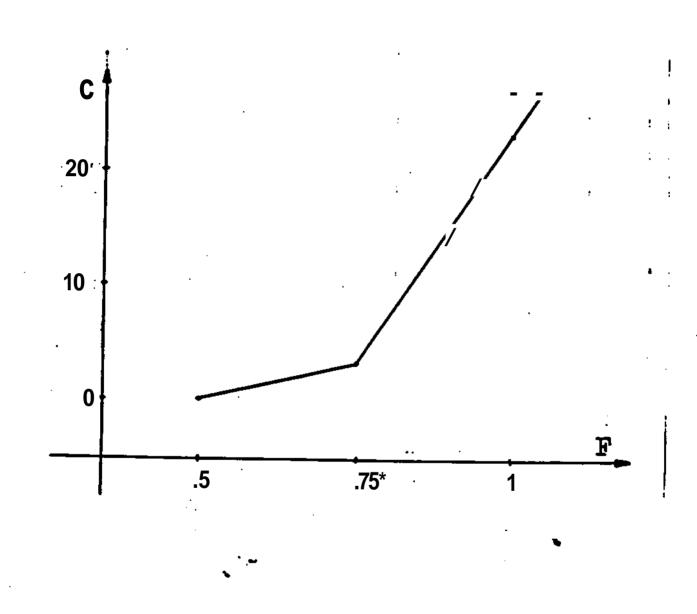


Figure 3: Coet vs. flexibility trade-off curve for example 1

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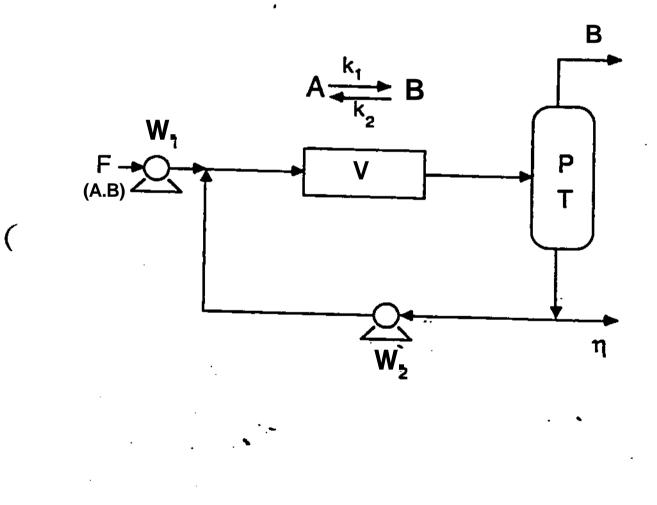
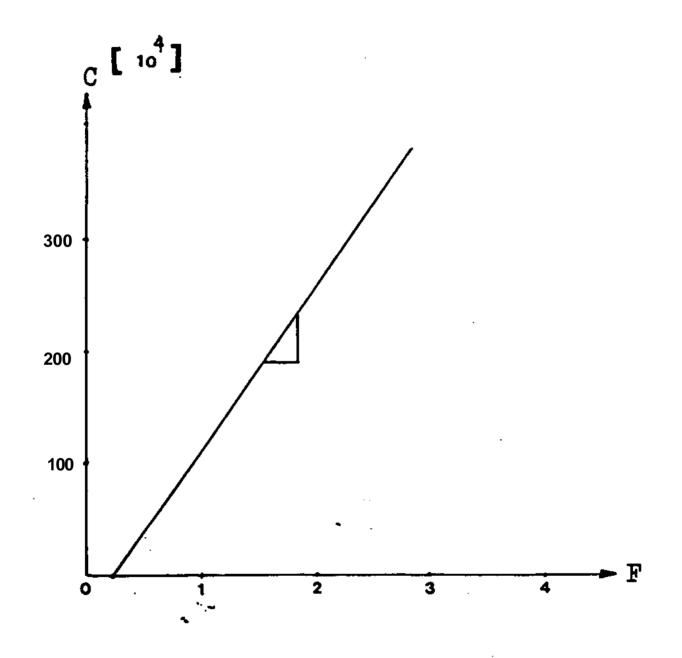
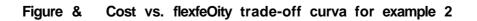


Figure 4: Proem** flowsheet for example 2

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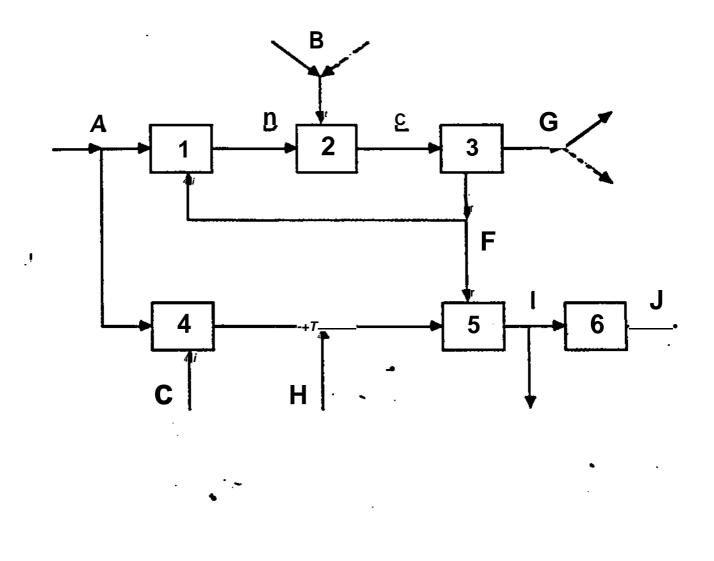


Figure ft Industrial chemical complex for example 3

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Table 1: Existing Design and cost data for example 2

Design variable	Existing value	Cost coefficient
V	7.5 m ³	10,000 \$/m³
w,°	22.0 kW	8,000 \$/kW
W ₂ ^D	15.5 kW	6,500 \$/kW

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Table 2: Economic data of chemical complex for example 3

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Investment cost (10*\$)

Process	Operating cost (\$/Kg)	fixed	variable
1	0.1	45.3	0.90
2	0.12	45.2	1.15
3	0.15	48.1	1.64
4	0.12	23.3	1.27
5	0.28	46.2	1.31
6	0.35	32.8	2.23
6 ^A	0.25	33.0	2.00

Table 3:	Existing	design	for	example		3
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design variable	capacity (Kg/hr)
d,	100
d ₂	150
d,	80
d₄	120
d,	100
d _e	40

Table 4:

Nominal values and deviations of the uncertain parameters in example 3

	(kg/hr)	(kg/hr)	(kg/hr)
Parameter	Nominal Value	Positive Deviation	Negative Deviation
*,	10	5	5
02	200	50	50
* 3	50	15	15
d_4	50	10	10
0 ₅	50	10	10

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