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Part II - Optimal Level of Flexibility

by

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IN NONLINEAR SYSTEMS
PART II - OPTIMAL LEVEL OF FLEXIBILITY

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ABSTRACT

In this paper the problem of establishing the optimal trade-off between investment cost for the retrofit and expected revenue that result from increasing flexibility in systems described by nonlinear models is addressed. A systematic procedure is first proposed for constructing the cost versus flexibility curve. A stochastic optimization method is then presented for evaluating the expected optimal revenue at a number of redesigns with specified degree of flexibility with which the trade-off curve relating expected revenue to flexibility is generated. This allows to identify the level of flexibility that maximizes the expected profit in a retrofit design. Examples are presented to illustrate the proposed strategy.

INTRODUCTION

In the first part of this series a novel computational strategy was presented for determining optimal retrofit designs with a specified fixed degree of flexibility in systems described by nonlinear models. The problem that will be addressed in this part is the one of finding the optimal level of flexibility that will maximize the total profit in an existing process flowsheet. The major issue in this problem is how to establish the optimal trade-off between investment cost for the retrofit and expected revenue that result from increasing flexibility.

In order to address the above problem two basic subproblems will be considered. The first one is the development of the trade-off curve relating flexibility to retrofit cost in the case of a chemical process whose performance is described by a nonlinear model. The major challenge here lies on how to avoid solving extensively the parametric optimization problem in terms of the flexibility index F. The second subproblem is the generation of the revenue curve as a function of flexibility. The challenge here lies on how to efficiently estimate the expected optimal revenue of the process given distribution functions for the uncertain parameters. It should be noted that these subproblems have been addressed by Pistikopoulos and Grossmann (1988b) for the case when a chemical process is described by a linear model. In this paper it will be shown that some of their basic ideas and solution strategies can be extended to the nonlinear case.

A systematic procedure is first proposed for constructing the curve that relates flexibility to retrofit cost. This procedure relies on identifying the break points of the different segments in the curve through the solution of NLP subproblems. These segments are characterized by different "limiting" sets of active constraints. From the trade-off curve a number of redesigns with specified degree of flexibility are obtained for which the corresponding expected optimal revenue is evaluated, it is shown that this can be performed through a modified Cartesian Integration method, that is coupled with the solution of NLP optimization problems.

PROBLEM STATEMENT

The specific problem which is to be addressed in the second part of these papers can be stated as follows:

The nonlinear model of an existing flowsheet with fixed equipment sizes and fixed structure is given which involves a set of uncertain parameters 0. Continuous distribution functions $p_i(0_i)$ i=1,.rP for the vector of the uncertain parameters are also specified. The nominal value 9^H of the uncertain parameters corresponds to the mean value, while positive and negative expected deviations $A0_r'$, Ad_i*, i•1,.,p are determined at a specified level of confidence. The problem is then to determine the required changes of the design variables d that will provide a flexibility that maximizes the total profit, consisting of the difference between expected revenue and retrofit cost.

In order to address this problem, two basic assumptions will be made:

1. The revenue of the process is strongly dependent on the uncertain parameters.

2. The expected revenue will be quantified over the feasible parameter space defined by the flexibility index F as introduced by Swaney and Grossmann (1985).

Also, for simplicity in the presentation no fixed charges will be assumed for the investment cost. Under these assumptions, this work will concentrate on firstly developing the retrofit cost curve and then estimating the curve of the expected revenue.

PROBLEM FORMULATION

For a fixed flexibility index F, the problem of determining minimum investment cost changes of the existing design can be represented in the following way if fixed charge costs are not considered:

$$C(F) = \min_{\Delta d} \sum_{i \in I} [\beta_i c(\Delta d_i)]$$

$$\text{s.t.} \quad \chi(d,F) = \max_{\theta \in T(F)} \min_{z} \max_{j \in J} f_j(d,z,\theta) \le 0 \qquad \text{(P1)}$$

$$d = d^E + \Delta d$$

where Δd_i, i=1,..,r, are the changes of the design variables to be determined for the existing design d^E. $\chi(d,F)$ is the feasibility function for a given design d for fixed flexibility F, and whose non-negative value implies feasible operation over the parameter range $T(F)=\{\theta \mid \theta^N - F\Delta\theta^- \le \theta \le \theta^N + F\Delta\theta^+\}$. As was shown in Part I, by introducing relaxation constraints for the function $\chi(d,F)$, problem (P1) leads to the following mathematical formulation:

$$C(F) = \min_{\Delta d} \sum_{i \in I} [\beta_i c(\Delta d_i)]$$

$$\text{s.t.} \quad \sum_{j \in J_A} \lambda_j^{k,\ell} f_j(d,z^{k,\ell},\theta^{k,\ell}) \le 0 \quad \ell=1,..,L, \; k=1...n_{AS} \qquad (P^L)$$

$$d = d^E + \Delta d$$

where n_{AS} corresponds to the number of potential active sets that limit flexibility, and L is the number of design points with associated critical points $\theta^{k,\ell}$ and multipliers $\lambda_j^{k,\ell}$ for each active set k. As was shown in Part I, problem (P^L) was incorporated within an algorithmic procedure for solving problem (P1). Clearly problem (P^L) is a parametric optimization problem in terms of the flexibility index

F. Consequently, in order to develop a trade-off curve of cost C(F) versus the flexibility F, problem (P^L) must be solved at a large number of values of F, and at each of these points feasible operation must be verified through problem (6) of Part I. It will be shown in the next section that a much more efficient computational scheme can be developed.

Also, if revenue considerations are taken into account, the problem of maximizing the expected profit Z with respect to flexibility can be represented conceptually in the following way:

$$\max_{Ad,F} \; Z = \underset{0GT(F)}{E} \left\{ \max_{z} \; riz.\$) \; | f(d,z,0)*O \right\} - \sum_{i=1}^{r} \beta_i c(\Delta d_i)$$

$$\text{s.t.} \quad X(d,F) \; £ \; 0 \qquad \text{(PO)}$$

$$d = d^E \bullet Ad$$

where Z is the profit as given by the difference between expected revenue and retrofit cost and r(z,0) is a nonlinear revenue function.

Problem (PO) is in general very difficult to solve, since it involves a stochastic semi-infinite nonlinear programming problem. For the linear case, Pistikopoulos and Grossmann (1988b) have proposed a systematic procedure to approximate problem (PO) by constraining the profit maximization to having minimum investment cost. This leads to a decomposition scheme which provides a good approximation to (PO) if the revenue of the process is strongly dependent on the uncertain parameters. If the revenue of the process is only function of the uncertain parameters, this decomposition scheme has been shown to be exactly equivalent to problem (PO). Using a similar line of reasoning for the case of nonlinear models leads to the following formulation:

$$\max_{F} \quad Z = R(F) - C(F)$$

$$\text{s.t. } C(F) = \min_{Ad} \sum_{j \in I} \beta_j c(Ad_j) \qquad \text{(P)}$$

$$\text{s.t. } \psi(d,F) \le 0$$

where the expected revenue R(F) is given by :

$$R(F) = \underset{\theta \in T(F)}{E} \{ \max_z \; r(z,\theta) \mid f(d,z,\theta) \le 0 \}$$

$$\text{s.t. } T(F) = \{ \theta \mid \theta^N - F\Delta\theta^- \le \theta \le \theta^N + F\Delta\theta^+ \} \qquad \text{(P2)}$$

$$d = d^E + Ad$$

$$Ad = \arg[C(F)]$$

In this way the solution of problem (P) can be decomposed in a similar way as for the case of linear models. First, problem (P1) has to be solved parametrically in F in order to determine the investment cost C(F) as a function of flexibility. Given then several fixed values of flexibility with associated design changes, the expected revenue curve R(F) is generated. Finally, a one dimensional search in the flexibility index F is performed to maximize the profit Z=R(F)-C(F). The difficulties that arise in the nonlinear case, however, stem from the two following points:

- In order to solve problem (P1) parametrically as a function of F, one can not resort directly to the parametric solution of problem (P^L) which in the linear case provides an exact representation.
- In order to estimate the optimal expected revenue for fixed flexibility an efficient integration scheme is required to handle nonlinear models.

In the next section both points will be addressed with the aim of developing efficient solution procedures.

TRADE-OFF CURVE OF COST vs. FLEXIBILITY

In this section it will be shown how the curve of retrofit cost versus flexibility, C(F), can be obtained. A typical trade-off curve is shown in Figure 1, which is a continuous piecewise nonlinear function consisting of a number of different segments (1-4, 4-3, 3-2 in Figure 1). Each segment is characterized by different "limiting" active sets of constraints, where their number increases with increasing flexibility index (see Pistikopoulos and Grossmann, 1988a). Therefore, break points (points 3 and 4) exist between adjacent segments. It then becomes clear that in order to construct such a curve it is first necessary to identify the sequence of break points in the curve, which will correspond precisely to the points where a change in the active sets of constraints that limit flexibility occurs.

The location of the break points will be identified by first determining the existing flexibility index (i.e. point 1 in Figure 1). Then an optimal redesign will be obtained with flexibility equal to the flexibility target F^T (i.e. point 2 in Figure 1). Based on the minimum cost solution at point 2, the next step will consist in determining the smallest value of flexibility for which the "limiting" active sets identified at point 2 remain the same. In this way point 3 in Figure 1 will be identified, which will correspond to a break point (kink) since a small move at a lower flexibility index value will give rise to different "limiting" active sets at minimum cost. Point 4 in Fig. 1 will be identified using a similar procedure. Finally, additional points between the break points can be generated to approximate the nonlinear curve in each segment with a polynomial function.

Based on the above discussion, a systematic procedure can then be proposed to generate the trade-off curve for nonlinear investment cost versus flexibility. It involves the following basic steps:

STEP 0 : At the existing design d^E, solve the flexibility analysis problem (eqtn. (4), Part I) to obtain the measure of flexibility $F^1=F^E$ and the corresponding n^1_s "limiting" active set(s) $AS^1(k) \mid J^1_A=\{j \mid f_j(d,z,\theta)=0\}, k=1,..,n^1_s\}$. Set $C(F^1)=0$.

STEP 1 : (a) Set $F^2=F^T$, where F^T is the maximum flexibility target up to which the curve is to be generated. Apply the procedure of Part I which involves the iterative solution of problem (P^L) for fixed flexibility F^2 to obtain the optimal design d^2 with cost $C(F^2)$ (i.e. at point 2 in the curve of Figure 1), and the corresponding n^2_{AS} "limiting" active sets $AS^2=\{k \mid J^Mj \mid f_j(d,z,0)=O\}, k=1,..,n^2_{AS}$h Set t=2.

(b) If AS^1 is identical to AS^1, go to step 3. Otherwise, go to step 2.

STEP 2 : (a) To identify a break point, define $J^k_{At}=\{j \mid f_j^k(d,z^k,0^k)=O\}$, $J^k_{Mt}=\{j \mid f_j^k(d,z\backslash 0^k) £ 0\}$, $k = I,..^*_{A5}$ where n^*_{A5} is the number of "limiting" active sets at point t, and z^k and 0^k are the control variables and uncertain parameters associated with the k'th active set. To determine the design d^{**1} with flexibility value F^{**1} where the closest break point occurs (e.g. point 3 in Fig. 1), solve the following optimization problem:

$$C(F^{'*1}) = \min_{Ad,F,\wedge^k} \sum_{i=1} [y?c(Ad)]$$

(P3)

$$\text{s.t.} \quad \left.\begin{array}{ll} f_j^{lt}(d,z^k,\wedge^{lt}) = 0 & j \in J^*_{At} \\ f_j^k(d,z^k\wedge^k) \leq 0 &]6 J^k_{Nt} \end{array}\right\} k=1,..,n^*_{AS}$$

$$d = d^E \cdot Ad$$

$$\theta^N - F\Delta\theta^- \leq \theta^k \leq \theta^N + F\Delta\theta^+$$

(b) Set F » F^{**1} - *t,* where « is a small positive number (i.e. <=0.02). Solve the feasibility test problem (eqtn. (6) of Part I) for d'^{*1} to identify new "limiting" active set(s) $AS"^1$ that are violated. Set t = t + 1 and go back to step Kb).

STEP 3 : Additional cost values between the break points can be generated by solving problem (P1) for a number of fixed flexibility values. However, note that the trade-off curve is characterized by the same "limiting" active sets between any adjacent points (e.g. points 1,4,3,2 in Fig. 1). If, in addition, the critical parameter points correspond to vertices, additional cost values can be generated for flexibility points F^{ℓ} between these adjacent points as follows: The number of active constraints describing each segment is $(n^t_{AS})x(n+1)$, where n is the number of control variables z. The total number of control variables z^k involved in the different active sets is $(n^*_{AS})x(n)$. Therefore, if the number of design changes Ad is equal to the number of active sets n^f_{AS} for the segment, as is often the case, then there are no degrees of freedom and additional cost values can be obtained through the solution of the following system of $(n^t_{AS})x(n+1)$ nonlinear equations in $(n^1_{AS})x(n*1)$ unknowns (control variables z\ and design changes):

$$J^k_{At} » \{ j \mid r^k_j(d,z^k,0) = 0 \} \quad k * 1,..,n^t_{AS} \qquad (1)$$

where $d=d^E+Ad$, and $0^k=0^N+FA0^f$, where A0* is the critical vertex direction. If the number of design changes Ad is smaller than n^*_{AS}, additional cost values are obtained through the solution of problem (P1) with $F*F^{\ell}$.

Note that the above algorithmic procedure systematically determines the active sets that characterize the different segments on the curve by efficiently detecting the sequence of their break points through the solution of problem (P3) in step 2(a), where the flexibility index F is treated as a free variable.

Also, it should be noted that in step 3 the reason why one can often determine additional points between adjacent break points through the system of nonlinear equations in (1) is that in most cases each active set can be modified through a single design change. Hence, for most cases the number of design changes will coincide with the number of active sets n^*_{AS} (see examples 1,2,3 later in the paper).

It should also be noted that in most cases there is an increase of only one new active set between any two adjacent segments. It then follows that if the number of design changes for this case is equal to the number of active sets in each segment, problem (P3) could be solved as a system of nonlinear equations, provided that the critical parameter values are vertices. The reason is as follows. Problem (P3) involves $n^t_{AS}x(n+1)$ equations. Since the flexibility index and the number of control variables is equal to $(n^*_{AS}xn)+1$, the degrees of freedom are consumed for $n^!_{AS}-i$ design changes. This corresponds precisely to the number of design changes at the kink if the **lower segment has** $n^\wedge_s$-1 active constraints. Clearly caution has to be exercised with this **scheme** since some of the inequalities in (P3) may be violated.

In the next section an analytical example of a small nonlinear problem will be presented to illustrate the steps of the proposed procedure to generate the trade-off curve of cost versus flexibility.

EXAMPLE 1

To illustrate the procedure in the previous section, consider that the specifications of a design are represented by the following inequalities:

$$f_1 = z^2/3 - (d_1 d_2 >< 9 \bullet d_i - 2d_2 £ 0$$

$$f_2 = -0.25(1,2 - 30/8 * d_2 \leq 0 \qquad (2)$$

$$f_3 = z * 0^2/5 - 2d_i - 2 £ 0$$

This nonlinear model was also studied in Part I (example 1), where an optimal redesign was obtained with flexibility, F^T=1. The existing design variables are d^^, d_2^E=3 and the values of the optimal redesign are d^T.B, d_2^T=4.88. The single uncertain parameter *0* has a nominal value 0^N=4 and expected deviations A#*=5, A0"=4. Applying the algorithmic procedure, the following results are obtained:

STEP 0 : At d^E*(4,3) the flexibility analysis problem yields F^1=F^E=0.585 with one "limiting" active set ASMJ. M(f.,f.)}}.

STEP 1 : (a) Set F^2=F^T=1.0. Then, the result obtained in Part I indicates that the optimal cost is 27.0 units (no fixed charges) with "limiting" active sets **AS^2={**J^-Mf/j)}, $J_A^{2=}${(f_2,f_3)H. Set t«2.

(b) AS^2 is not identical to AS^1. Go to step 2.

STEP 2 : (a) Problem (P3) can then be formulated in the following way:

$$\min_{F,\Delta d_1,\Delta d_2} \quad 5\Delta d_1^{+} \cdot 5\Delta d_2^{+}$$

s.t. $f_1^1 = \langle z V - \wedge \text{-} d_1)*^1 \cdot d_1 - 2d_2 = 0$

$f_2^1 * -0.25d_1(z^1) - (3/8)0^1 \cdot d_2 \gg 0$

$f_3^1 = (z^1) * (0^1)^2/5 - 2d_1 - 2 * 0$ (3)

$f_2^2 = -O\wedge Sd/z^2) - (3/8)\wedge^2 * d_2 = 0$

$f_3^2 = (z^2) * (0^2)^2/5 - 2d_1 - 2 = 0$

$f_1^2 = (z^2)^2 - \{6_j\text{-}4_2)6^2 \cdot d_1 - 2d_2 \wedge 0$

$d_1 = 4 + \Delta d_1$

$d_2 * 3 \cdot \Delta d_2$

$\Delta d_1 = \Delta d^\wedge - \Delta d/, \ \Delta d_2 = \Delta d_2^* - \Delta d_2^*$

$\Delta d_1 \backslash \Delta d; _f \Delta d_2 \backslash \Delta d_2' \wedge \quad 0$

$\theta^N - F\Delta\theta^- \leq \wedge^k \wedge 9'' + ?\Delta d \backslash \quad k=1,2$

The solution of the above problem (3) yields F=0.898, Δd_1=2.144, Δd_2=0.0; i.e. the break point occurs at a value of F^3=0.898, which corresponds to a redesign with d^e.144, d_2=3, at a minimum cost of 10.72 units. Note, that if the design change Δd_2 is fixed at a value of zero, then problem (3) can also be solved as a system of four equations (f_1^1, f_2^1, f_2^2, f_3^2) in four unknowns (F, Δd_1, z^1, z^2), with $0^1=0^N$-4F and $0^2=0^N$+5F. This follows from the fact that the number of "limiting" active sets at F^2 is two, while there is only one "limiting" active set at F^1.

(b) Set F=0.898-0.008=0.89 (e =0.008). Then the feasibility test problem can be formulated as follows for the two potential sets of active constraints:

$$*^k(d,F) = \max_{u,z^r,0} u$$

s.t. $f_j^k = u \qquad j \in J_\wedge^k, \ k=1,2$ (4)

$0.44 \wedge 8 \leq 8.45$

$$F = 0.89, \; d \approx (6.144,3)$$

where J_A^1*f(f_1,f_2)} and J_A^2={(f_2,f_3}. The solution of problem (4) yields X^O, $*^2$=1.58>0. Therefore, the -new "limiting" active set for the next segment is AS^3={J_A^2={(f_2,f_3n. Set t*3 and go back to step Kb).

STEP 1 : (b) Since AS^3 is identical to AS^1 there are no other break points, go to step 3.

STEP 3 : The curve consists of two segments as seen in Figure 2. Additional points can be generated by considering several additional flexibility points F^ through the solution of the following system of equations describing each segment

SEGMENT 1-3

$$f_2^2 = -O\text{^}Sd/z^2) - (3/8M0^N+5F\text{^}) + 3 » 0 \qquad (5a)$$

$$f_3^2 = (z^2) \bullet <0^N+5F^£)^2/5 - 2d, - 2 » 0$$

SEGMENT 3-2

$$f,^1 = (z^1)^2 - (d_r d_2)(0^N-4F^£) \bullet d, - 2d_2 = 0$$

$$f_2^1 = -0.25d,(2') - (3/8)(\text{^}^N-4F\text{^}) + d_2 = 0 \qquad (5b)$$

$$f_2^2 * -0.25d_1 (z^2) - (3/8)(\text{^}^N+5F^£) \bullet d_2 = 0$$

$$f_3^2 = (z^2) * (0^N+5F*)^2/5 - 2d_l - 2 = 0$$

By evaluating the cost for the corresponding design changes, and fitting a polynomial, leads to the curve shown in Figure 2.

EXPECTED REVENUE

In order to motivate the proposed procedure for estimating the expected revenue, consider a nonlinear revenue function *r(z.d)=z+d²* in the previous example. Also assume a normal probability distribution function p(0) for the single uncertain parameter of the form N(4,4). With a level of confidence of 86% for the positive expected deviation and 70% for the negative expected deviation, their values are A0*=5 and A0"*4 respectively.

For the existing design d^E, which has a flexibility index F^E=0.585, we can evaluate the maximum revenue at different fixed values of *d* in the range $T(F^E)$={0 | 1.66S0S6.925} by solving the NLP problem:

$$\max_z \quad z \bullet d^2 \qquad (6)$$

$$f_l = z^2/3 - (d_1^E - d_2^E)0 * d_1^E - 2d_2^E £ 0$$

$$f_2 = -0.25d_1^E z - 3(9/8 \bullet d_2^E £ 0$$

$$f_3 = z \bullet 0^2/5 - 2d_1^E - 2 £ 0$$

where d_1^E=4, d_2^E=3.

In order to construct a piecewise linear approximation of the maximum revenue as a function of *6,* assume that problem (6) is solved at the following four points: the nominal value 0^N=4, the lower bound 0^L=1.66, the upper bound 0^U=6.925, and the optimal value of *8* corresponding to the highest revenue if *6* is an interior point within the range T(F)=T(0.585). This latter point is obtained from (6) by treating *d* as an additional variable for the optimization. The results obtained are summarized in Table 1, where it can be seen that the fourth point coincides with the upper bound. Having obtained the three revenue values *r{$J.* $r(0_2)$, $r(0_3)$ in Table 1 the segments between them are approximated with the linear functions *rt^d)* and *rljd);* where *rl^(d)* * *[riej-riOJHOfe^e* • *WO)6$_2$-T(8}0JIO$_2$-S$_y$Y^y* and a similar expression holds for $rl_2(0)$. Figure 3 shows the piecewise approximation of the optimal revenue function that is obtained. This Figure also shows the actual nonlinear curve obtained through the solution of a large number of parameter points. The error of the piecewise approximation in this case is of the order of less than 4%.

Using the piecewise linear aproximations the optimal expected revenue at the existing flexibility F^E can be obtained by integrating over *S* as follows:

$$R(F^E) = \int_{\theta^-_1}^{\theta^+_3} r(\theta)\, p(\theta)\, d\theta = \int_{\theta^-_1}^{\theta^+_1} r(\theta) p(\theta) d\theta + \int_{\theta^-_2}^{\theta^+_3} r(\theta)\, p(\theta) d\theta = 24.056 \qquad (7)$$

In order to obtain values of the expected revenue R(F) at two other flexibility values, the points F=0.898 and F=1.0 were considered. Table 2 summarizes the results obtained for the three designs. By fitting a polynomial for the three expected revenue values the curve shown in Fig. 4 is obtained. Plotting also the trade-off curve generated previously in Fig. 2, the curve for the total profit is obtained. Note that the optimal flexibility results at the value F*=0.898 (i.e. the break point) with corresponding design values d=(6.144,3.0), which only implies a change in the first design variable of Ad^2.144. Note that the predicted expected profit of this redesign is 30 units, which represents an increase of 25% of the expected profit of 24 units for the existing design.

This example involved only one single uncertain parameter *d* and hence the procedure for estimating the expected revenue is relatively straightforward. Also note that at each of the three flexibility values chosen, only 4 NLP's (eqtn (6» had to be solved. In the case when 2 or more uncertain parameters are involved, however, a special method must be devised to estimate the multiple integral of the expected revenue so as to minimize the number of NLP subproblems to be solved.

In the next two sections a summary of the Modified Cartesian Integration method will be first presented, which is a direct extension of the one discussed in detail for the linear case (see Pistikopoulos and Grossmann, 1988b, and Bureanu, 1980). Then the piecewise linear approximation for the evaluation of the conditional optimal expected revenue function will be presented for the general case.

MODIFIED CARTESIAN INTEGRATION METHOD

The basic idea of the Cartesian Integration method (Bureanu, 1980) is to approximate the multiple integral of the expected revenue through Gaussian quadrature of n^-1 uncertain parameters, and to evaluate one-dimensional analytical integrals in terms of a single uncertain parameter d_m at each of the nodes of the quadrature formula. However, since the number of nodes that must be considered for the n^-1 parameters in the Gaussian quadrature formula increases very rapidly, the vector of the uncertain parameters will be partitioned in order to select only few uncertain parameters for which nodes will be considered in the Gaussian quadrature formula. This has the important effect of reducing the number of NLP problems to be solved. This Modified Cartesian Integration method, which is described in detail in Pistikopoulos and Grossmann (1988b), consists of three major steps:

STEP 1. Partitioning of the vector *8* of the uncertain parameters in three subsets according to their economic sensitivity: *6* , a single independent parameter that exhibits the largest sensitivity to the revenue; ff_{Qf} a vector of dimensionality D£1 with significant sensitivities to the revenue; and B_s, the remaining uncertain parameters of dimensionality S whose sensitivity to the revenue can be neglected. Discretization of the subset d_Q is performed at a finite number of nodes q, q€Q, corresponding to the roots of the Gaussian quadrature formula (see Carnahan *et a/,* 1969).

STEP 2. Evaluation of the conditional expected revenue function $R_q(F)$ at each node q through a one-dimensional integral in d_m (see eqtn (11) in next section).

STEp 3. Estimation of the expected revenue from the following expression (see Bureanu, 1980):

$$R(F) = M \sum_{q \in Q} IT \; w \; R(F) TT^{D}{}_{i} p(^{\wedge q}) \qquad (8)$$

where M * T° TT^{D} {$ ^{u}-0 ^{L})

I I i ' i Di Di

w_q = weight for Gaussian quadrature at node q

$R_q(F)$ = conditional expected revenue for θ_m and θ_s at node q

θ_{Di}^{q} ... [illegible]

t_i = roots of the Gaussian quadrature formula

Since steps 1 and 3 are essentially equivalent to the ones for the linear case, only step 2 will be presented in some more detail for the nonlinear case, where a piecewise linear approximation of the nonlinear conditional expected revenue is applied.

EVALUATION OF THE CONDITIONAL EXPECTED REVENUE FUNCTION

At each node q, the conditional expected revenue function $R_q(F)$ at the flexibility value F will be of the following form (see Pistikopoulos and Grossmann, 1988b):

$$R_q(F)=\left[\int_{\theta_m^L}^{\theta_m^U} (\max_z \; r(z,\theta_m, \theta_S^q, \theta_D^q)) p(\theta_m) d\theta_m\right] \left[\int_{\theta_S^L}^{\theta_S^U} \prod_{i=1} p_i(\theta_{S_i}) d\theta_S\right] \quad (9)$$

In order to evaluate the above integral, which is separable in θ_m and θ_S, the integration of the optimal expected revenue in θ_m has to be obtained in a similar fashion as was obtained for the small nonlinear example that was discussed previously. At a given value of θ_m, the optimization of the revenue function will be given by:

$$T(\theta_m) = \max_z \; r(z, \theta_m \mid \theta_S^q, \theta_D^q)$$

$$\text{s.t.} \quad f(d,z,\theta_m,\theta_S^q,\theta_D^q) \le 0 \quad (10)$$

where d corresponds to the design determined at the given value of the flexibility index F. **The idea** is then, as in the small example, to approximate the optimal revenue function as a piecewise linear function considering essentially four uncertain parameter values and the corresponding optimal values of the revenue function through the solution of problem (10). The four parameter values that are selected are: the nominal point $6_{mm}^{1}=8^{N}$, the lower bound $6_{mm}^{2}=8^{L}$, the upper bound $8_{mm}^{3}=0^{u}$ and the optimal point $8_{mm}^{A}=8^{*}$ obtained from (10) with 0_{m} as an additional optimization variable. The point 8_{m}^{A} is only considered for the piecewise approximation if it is an interior point within the range $[8^{L}_{mm}, 8^{U}L$ In this way, the conditional expected revenue function can be approximated in the following way:

$$R_q(F) = [T_{*-*}^{3} \int_{J_m}^{a_m^{n*i}} rl_k(9)p_{mm}(8_{mm})d9] [\int_{J_S}^{a_S^{u}} TTP_{Si} <*_{Si} \wedge_{Si}] \qquad (11)$$

where $x/_{km}\backslash 8)$ is the linear approximation function for each segment $[8 \backslash 6_{mm}^{k*l}]$ and is given by the following expression:

(12)

$$\backslash\backslash_{km}, \backslash yj \; I - L'\backslash_m \; I \; r\backslash(7_m \; I \; J \; L_m \; {}_m \; J \; "_m \; L'\backslash" \; /C7_{mm} \; \backslash\backslash U_{mm} \; IU \; J \; L \; "_{mm} \; J$$

where $r(8_m^k)$ is the optimal objective function value of (10) at the parameter point 8_m^k, k=1,2,3,4.

Finally, the curve of the expected revenue R(F) as a function of F is generated by fitting a polynomial over a specified set of flexibility values where the expected revenue is evaluated.

ALGORITHMIC PROCEDURE TO IDENTIFY OPTIMAL FLEXIBILITY

Based on the analysis presented in the previous sections an algorithmic procedure can then be developed to determine the optimal degree of flexibility while redesigning an existing chemical plant with a nonlinear model. It involves three steps:

STEP 1 : (a) Construct the retrofit cost versus flexibility trade-off curve C(F) by applying the procedure described previously in the paper.

(b) From the curve select a set of N+1 flexibility values $\{F^1\}$ and the corresponding set of design variable values $\{d^1\}$.

STEP 2 : (a) For each value of flexibility F^1 and its associated design variable d^j, estimate the expected revenue R(F') as given by equation (8). This step involves the procedure for approximating the conditional expected revenue that was described in the previous section.

(b) Using polynomial approximation, fit a curve for R(F) using the points [F',R<FU

STEP 3 : Given the curves for R(F) and C(F) determine with a one-dimensional direct search procedure the degree of flexibility $F^{\#}$ that maximizes Z=R(F)-C(F).

In the next section two process example problems will be considered to illustrate the application of the proposed procedure.

EXAMPLE 2

Example 2 corresponds to the nonlinear model of the chemical process flowsheet shown in Figure 5, that involves a PFR reactor, a fractionator and a recycle stream. A slightly modified version of this flowsheet problem was studied for the linear case in Pistikopoulos and Grossmann (1988a).

The existing design of the flowsheet has a volume of the reactor V=7.5 m^3 and limits for the powers of the two pumps W_1^D=22.O KW and W_2^o=15.5 KW, respectively. Three uncertain parameters are involved in the description of this system: the composition of B in the feedstream (0,) and the reaction rate constants k_i *{0J* and k_2 (0_3). Distribution functions are provided for the three uncertain parameters, as shown in Table 3, and the corresponding nominal values as well as the expected deviations for a confidence level of 85% for both directions.

Retrofit cost data and the nonlinear revenue function, accounting for profit from sales, cost of raw material and operating cost, are also listed in Table 3. The problem is then to determine the degree of flexibility that maximizes the total profit, consisting of the difference between expected revenue and cost for the necessary modifications.

The flexibility index of the existing design is F^6=0.50 with one "limiting" active set $AS^1=\{J_A^1\}$ consisting of four constraints, since three control variables are involved (the pressure P and the temperature T of the separation column, and the flowrate of the feedstream F). One active constraint is the purity requirement for the product B, whereas the remaining three are simple bounds for the temperature T and the actual work required by the two pumps. Setting the flexibility target to F^T=1.O, and applying the procedure of Part I, yields a reactor volume increase of 6.5 m^3 with a minimum cost of $130,000/yr in order to achieve a redesign with the required flexibility. The "limiting" active set at F^T is again AS^1, which implies that no break points occur, and hence the curve is characterized throughout by the same active set. By considering a number of other points F^ within [0.5,1.0] and solving the system of nonlinear equations describing active set J_A^1 in AV the corresponding cost values are obtained, with which the trade-off curve is then generated as shown in Fig. 6.

From the cost curve three points, F^j={0.5, 0.82, 1.0} with corresponding design variables d^j={(7.5,15.5,22.0), (10.0,15.5,22.0), (14.0,15.5,22.0)} are selected to construct the curve for the expected revenue. Optimizing the existing design at the nominal parameter values, the sensitivity coefficients that were obtained for the uncertain parameters (see Pistikopoulos and Grossmann, 1988b) are:

$$[\ r_1 = 2673,\ r_2 = 858,\ r_3 = 572\ ].$$

Since $r_1 > r_2 > r_3$, the fraction of B in the feedstream (θ_1) is selected as the independent uncertain parameter, whereas the two kinetic constants are both selected to be discretized. Thus:

$$[\ \theta_m = \theta_1,\ \theta_D = (\theta_2,\theta_3),\ \theta_S = \emptyset\ ]$$

Selecting three points for each uncertain parameter $\theta_{D,i}$, i=1,2 nine nodes were generated for the integration. At each node four optimization problems were solved for constructing the piecewise approximation of the conditional expected revenue. Since three values of fixed flexibility were selected, a total of 108 NLP optimization problems were solved overall in order to estimate the expected revenue at the three redesigns. The results are summarized in Table 4. Figure 6 shows the resulting revenue curve as well as the optimal flexibility of $F^{\#}$=0.87, with a corresponding optimal profit of 1.75x10^5 \$/yr. At this point solving problem (P1), yields an increase in the reactor volume of 4 m^3. Therefore, by increasing the reactor volume from 7.5 m^3 to 11.5 m^3 the expected profit of the process flowsheet in Fig. 5 can be increased from 0.74x10^5 \$/yr to 1.75x10^5 \$/yr due to the increased flexibility from the existing index 0.5 to the optimal value of 0.87.

EXAMPLE 3

A slightly modified version of the reactor system considered in Halemane and Grossmann (1983) and Pistikopoulos and Grossmann (1988b) is shown in Figure 7, which consists of a reactor-cooler system, where a first order exothermic reaction A → B takes place. The existing design of this flowsheet has a volume of the reactor V=4.6 m^3 and an area of the heat exchanger A=12.0 m^2. Two uncertain parameters will be considered, the feedflowrate, F_o and the reaction rate constant k_o. Distribution functions, the corresponding nominal values as well as the expected deviations for a confidence level of 85% are shown in Table 5, where retrofit cost data and the nonlinear revenue function are also listed. The specification constraints and the nonlinear model of this process can be found in Pistikopoulos and Grossmann

(1988b).

The flexibility index of the existing design is F^E=0.05, due to the large expected deviations. The trade-off curve of cost versus flexibility can then be generated by applying the algorithmic procedure that was described in this paper and is shown in Figure 8. Note, that no break points occur and the solution indicates that only one design modification is required, a reactor volume increase with corresponding values depending on the level of flexibility, as shown in Table 6, where the associated costs are also listed.

In order to generate the curve for the expected revenue, three points were considered for the flexibility $\{F^i\} = \{0.05, 0.5, 1.0\}$ with the corresponding design variables $\{d^i\} = \{(4.6,12.0),(5.54,12.0),(6.644,12.0)\}$. The sensitivity analysis, for the existing design and nominal parameter values, results to the following partitioning for the two uncertain parameters: $d_m = 0_1 = F_o$, $8_D = 0_2 = k_o$, $0_S = 0$ (since r_1 =23.2 > r_2 =0.15). Selecting four nodes for d_Q and applying the procedure for estimating the expected revenue at each value of F^1 yields the results shown in Table 6, obtained through the solution of 48 NLP optimization problems. Then the optimal profit curve is generated, as shown in Figure 9, where it can be seen that the optimal flexibility is at a value $F^{\#}$=0.733, corresponding to a redesign with V=6.0 m^3, A=12.0 m^2 and a maximum expected profit of 140,000 $/yr.

Finally, it is interesting to compare the above result with the case when the redesign is performed at only one condition; e.g. maximize profit at the "worst" point (high F_o, low k_o) for a given flexibility index. The results are shown in Table 6. As it can be seen, the redesign with F=1 has a higher profit (242.2x10^3 $/yr) than the one of the existing design with F^E=0.05 (7.2x10^3 $/yr) and higher than the one of the redesign with F=0.733 (185.8x10^3 $/yr). Thus, one might be tempted to select the design with flexibility F=1. However, note that this profit was only evaluated at the worst condition. If on the other hand expected revenue considerations are taken into account, as it was shown in this example with normal probability distribution functions describing the two uncertain parameters, the redesign with F=0.733 is in fact the optimal one. Thus, this result shows the importance of properly evaluating the expected revenue, and hence the expected profit for a retrofit design.

CONCLUSIONS

In this paper the problem of establishing the optimal trade-off between retrofit cost and expected revenue for increasing flexibility in a chemical process has been addressed. First, by considering a nonlinear model for the process, an efficient algorithmic procedure has been developed to generate the trade-off curve relating retrofit cost to flexibility, and which avoids the need of solving extensively the resulting parametric nonlinear optimization problem. This procedure consists in systematically identifying the break points in the curve by detecting the active sets of constraints that provide a limit on the increase of flexibility. Then, by considering probability distribution functions for the uncertain parameters, the optimal increase of flexibility that maximizes the total profit of the chemical process can be evaluated by generating the expected revenue curve as a function of flexibility. An extension of the algorithmic procedure developed by the same authors for the linear case has been presented for this case, which is based on approximating the conditional optimal revenue as a piecewise linear function. The efficiency of the proposed methods has been illustrated with three example problems.

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Table 1: Expected revenue approximation data for example 1

	0	*r(8)*
nominal value (0^1)	4.0	20.2426
lower bound (0^2)	1.66	6.0692
upper bound (0^3)	6.925	48.364
optimal value	6.925	48.364

Table 2: Cost Expected revenue and profit values for example 1

Flexibility index	Design variable	Cost function	Revenue function	Profit ••
F	d	C(F)	R(F)	2
0.585	(4,3)	0.0	24.056	24.056
0.898	(6.144,3)	10.72	40.6566	29.936
1.0	(7.501,4.878)	27.0	48.367	21.367

Table 3: Data for uncertain parameters, cost and revenue function for example 2

Uncertain Parameter	Distribution Function	Nominal Value	Positive Deviation	Negative Deviation
e	•	*e"*	*Ad**	*Ad'*
c_B	N(0.5,0.02)	0.5	0.03	0.03
k, ls"[1])	N<0.02,0.002)	0.02	0.003	0.003
k_2 (s^{-1})	N(0.01,0.0008)	0.01	0.001	0.001

Retrofit cost: 2 AV + AW^ • AW_2^D ($\$10^4$/yr)

Revenue : r = 500 F_4 * 150 F_6 - 180 F - 0.1 F_3(900-T) ($\$10^6$/yr)

Table 4: Cost Expected revenue and profit values for example 2

Flexibility index	Design variable	Cost function	Revenue function	Profit
F	d (m^3,KW,KW)	C(F) $\$10^4$/yr	R(F) $\$10^5$/yr	Z $\$10^4$/yr
0.5	<7.5,15.5,22)	0	0.74	7.4
0.82	(10,15.5,22)	**5**	2.19	17.0
1.0	(14,15.5,22)	13	2.95	16.5

Table 5: Data for uncertain parameters, cost and revenues for example 3

Uncertain Parameter	Distribution Function	Nominal Value	Positive Deviation	Negative Deviation
θ	••	θ^N	A<T	*Ad'*
F_0 (Kmol/hr)	N(45.36.18.O)	45.36	22.68	22.68
k_o (hr^{-1})	N(12.0,0.8)	12.0	1.2	1.2

Retrofit cost: 200 AV + 80 AA ($\$10^3$/yr)

Revenue function: r = 100 F_Q - (10 F_1 + 5 FJ <$\$iO^3$/yr)

Table 6: Cost, Expected revenue and profit values for example 3

Flexibility index	Design variable	Cost function	Revenue function	Profit at worst point
F	d (m^3,m^2)	C(F) $\$10^3$/yr	R(F) $\$10^3$/yr	$\$10^3$/yr
0.05	(4.6,12.0)	0.0	9.39	7.2
0.33	(5.162,12.0)	130	..	..
0.50	(5.537,12.0)	200	304.74	115.2
0.75	(6.0,12.0)	280	420.0	185.8
1.0	(6.644,12.0)	405	**516.72**	242.2

FIGURES

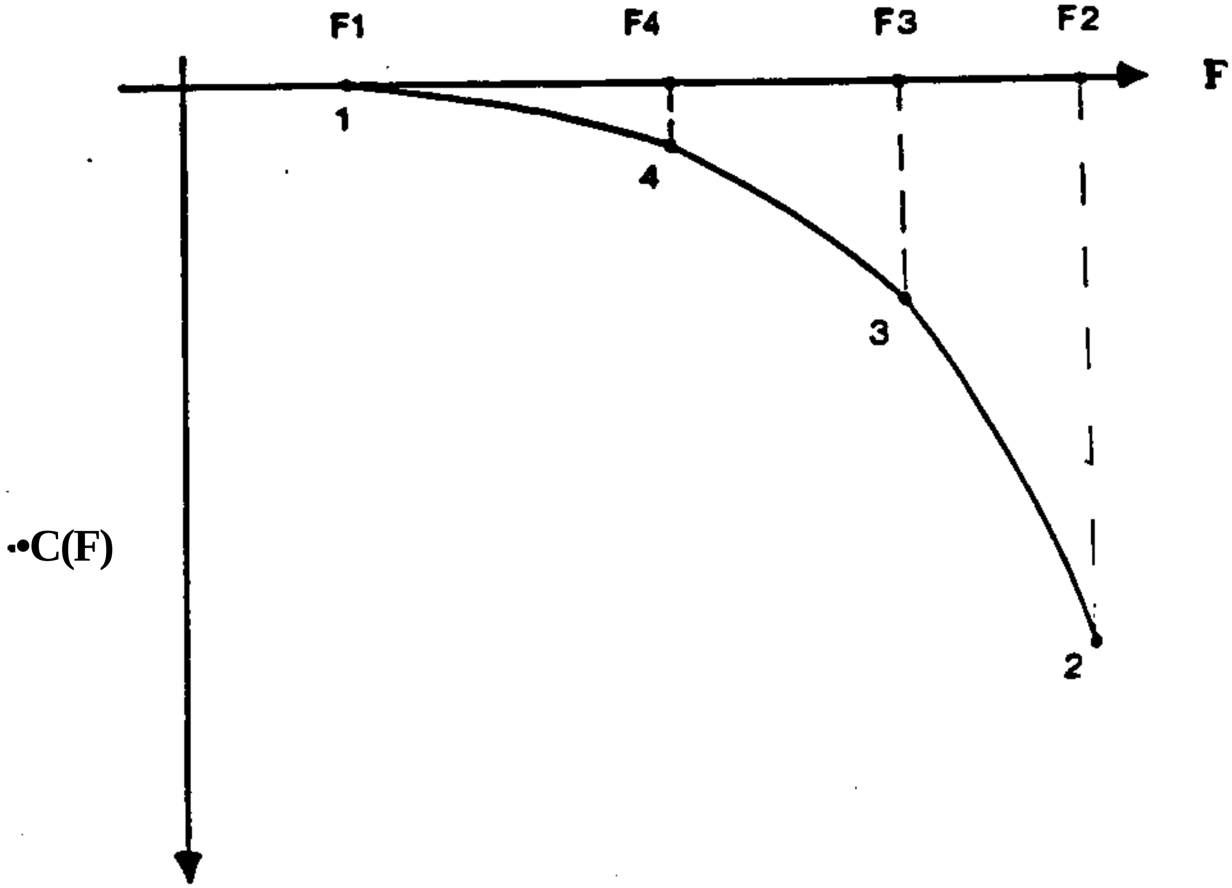

Fig. 1

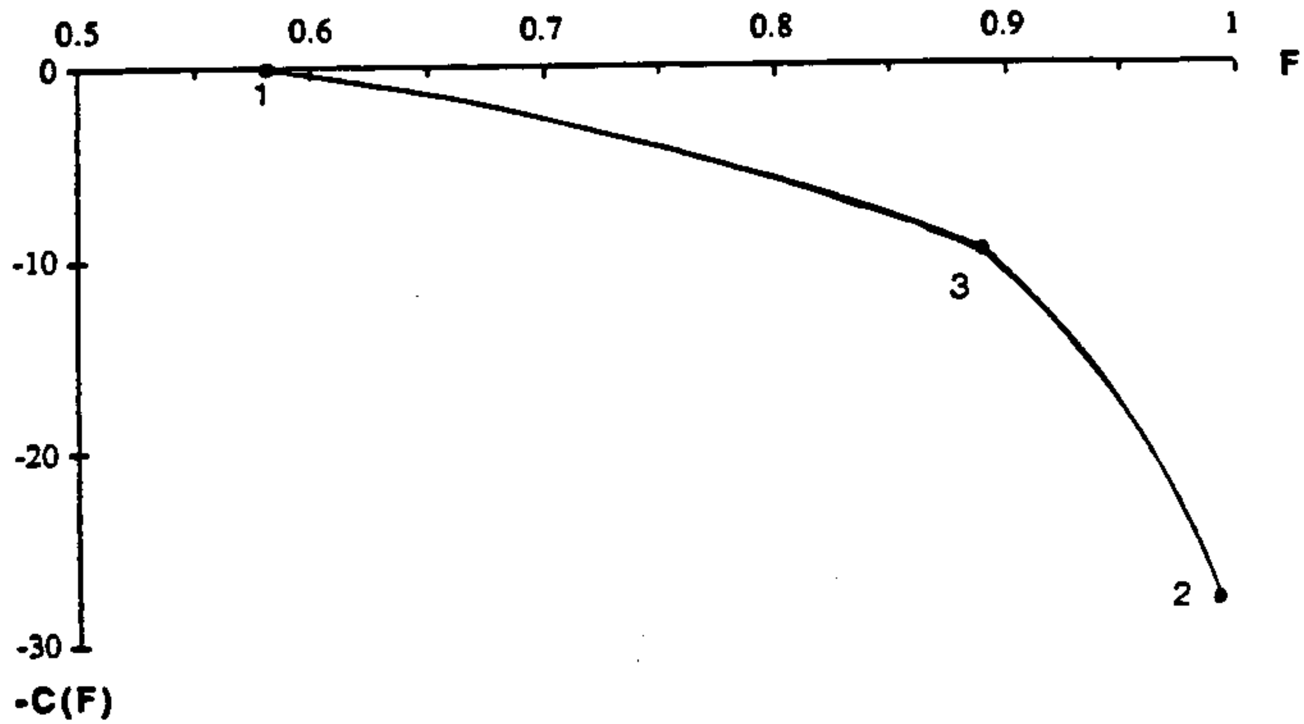

Fig. 2

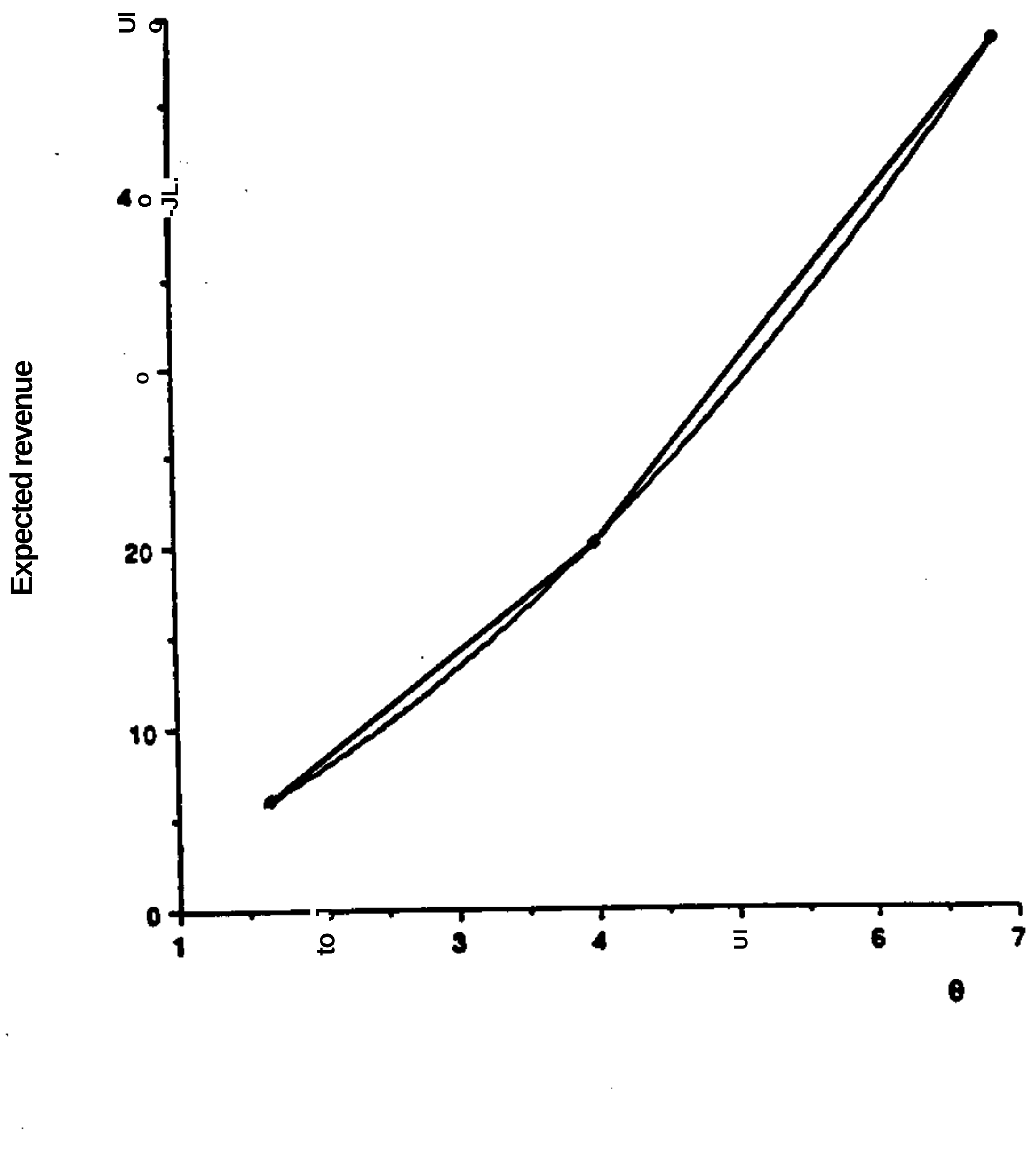

Fig.

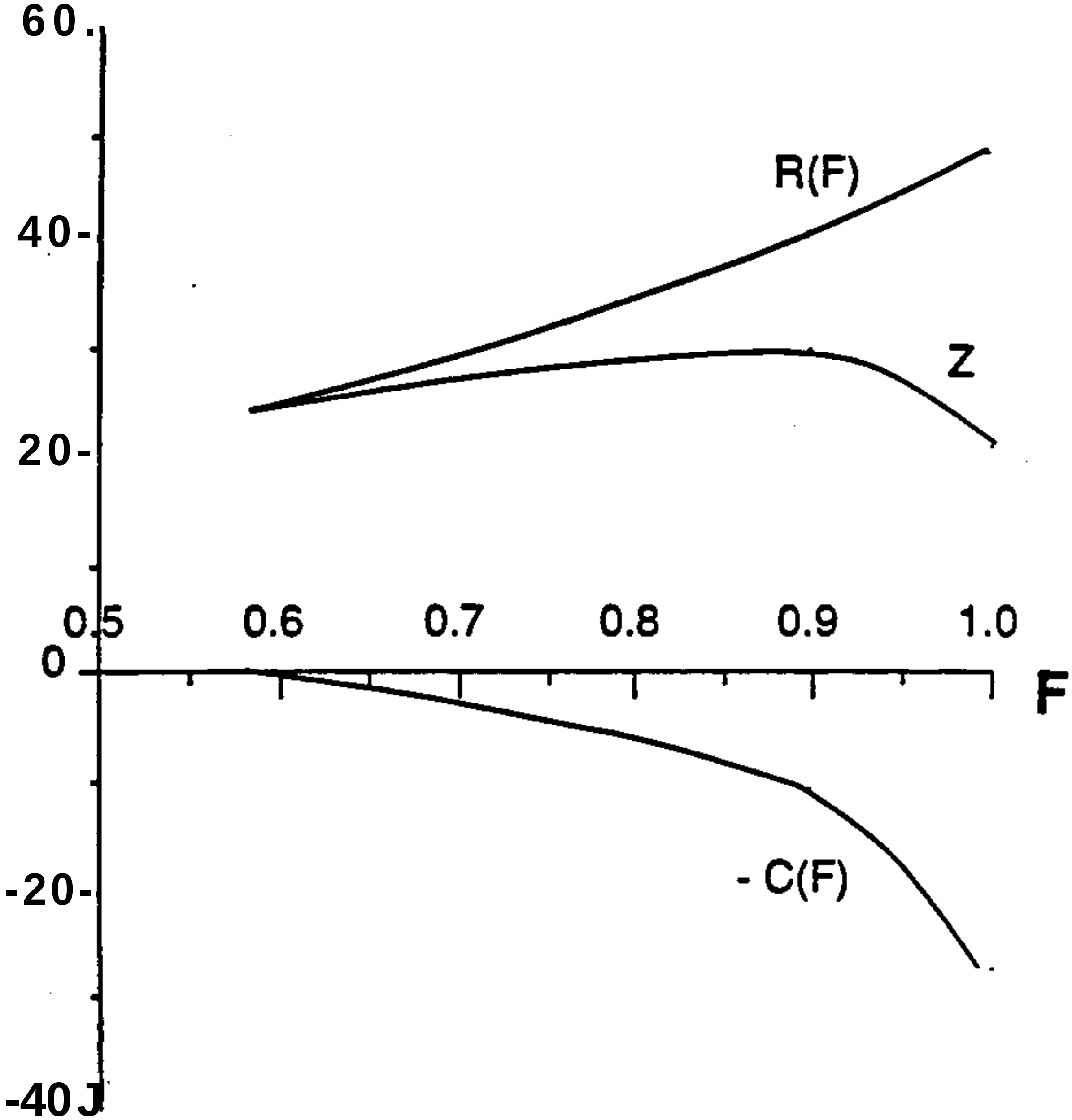

Fig. 4

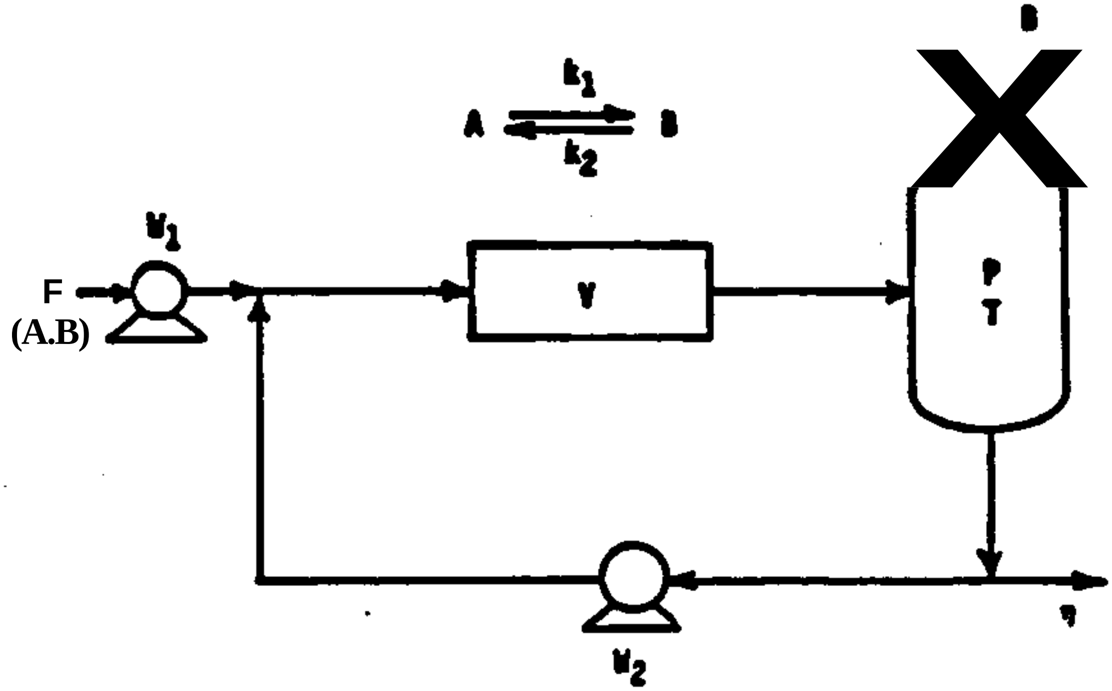

Fig. 5

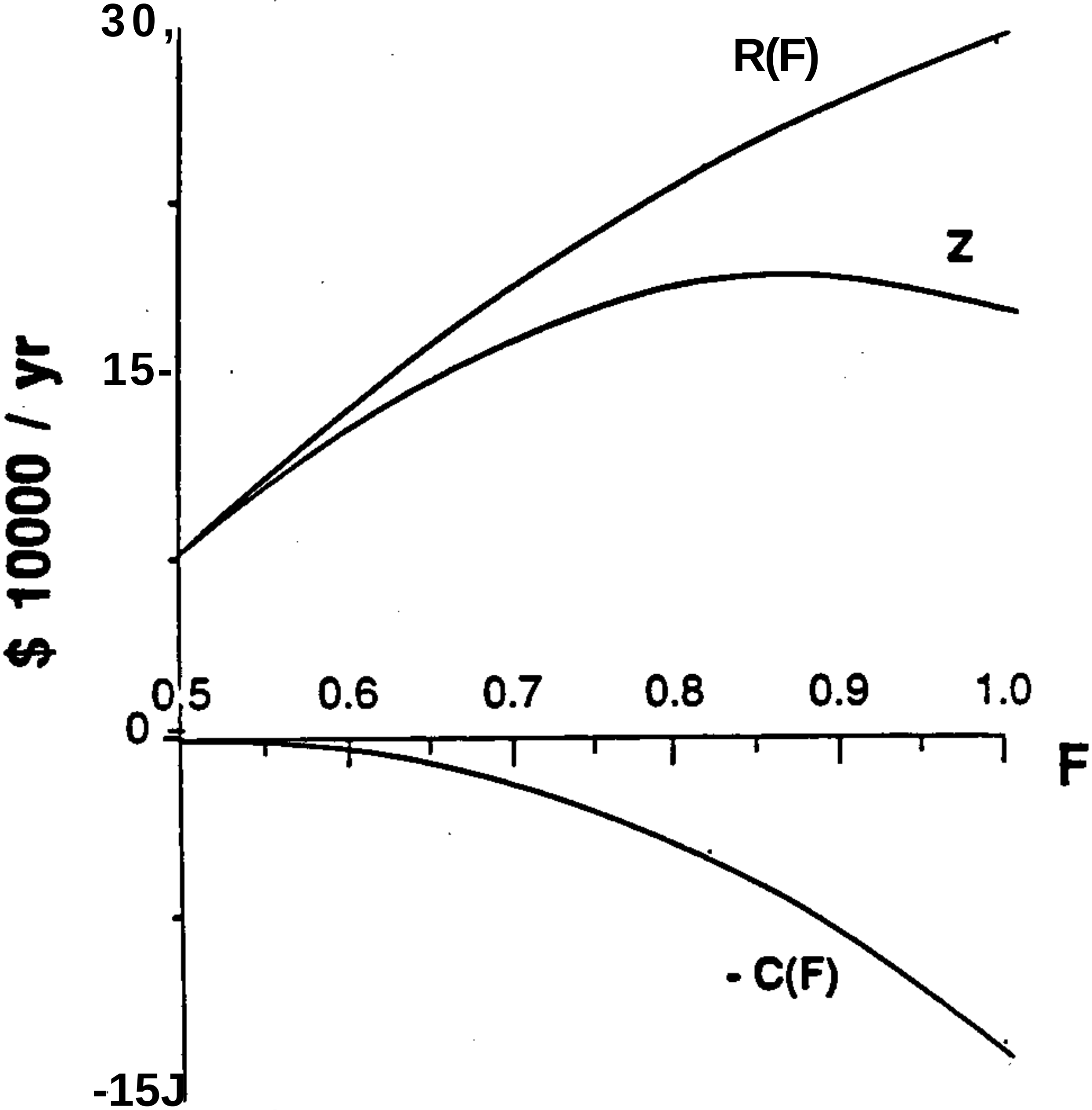

Fig. 6

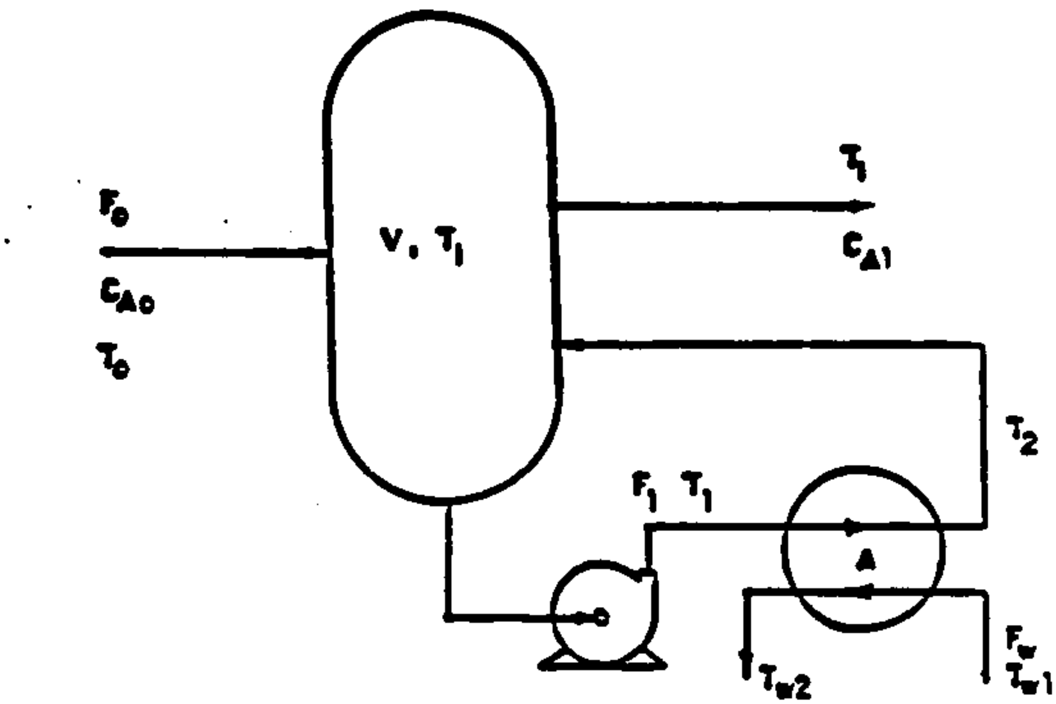

Fig. 7

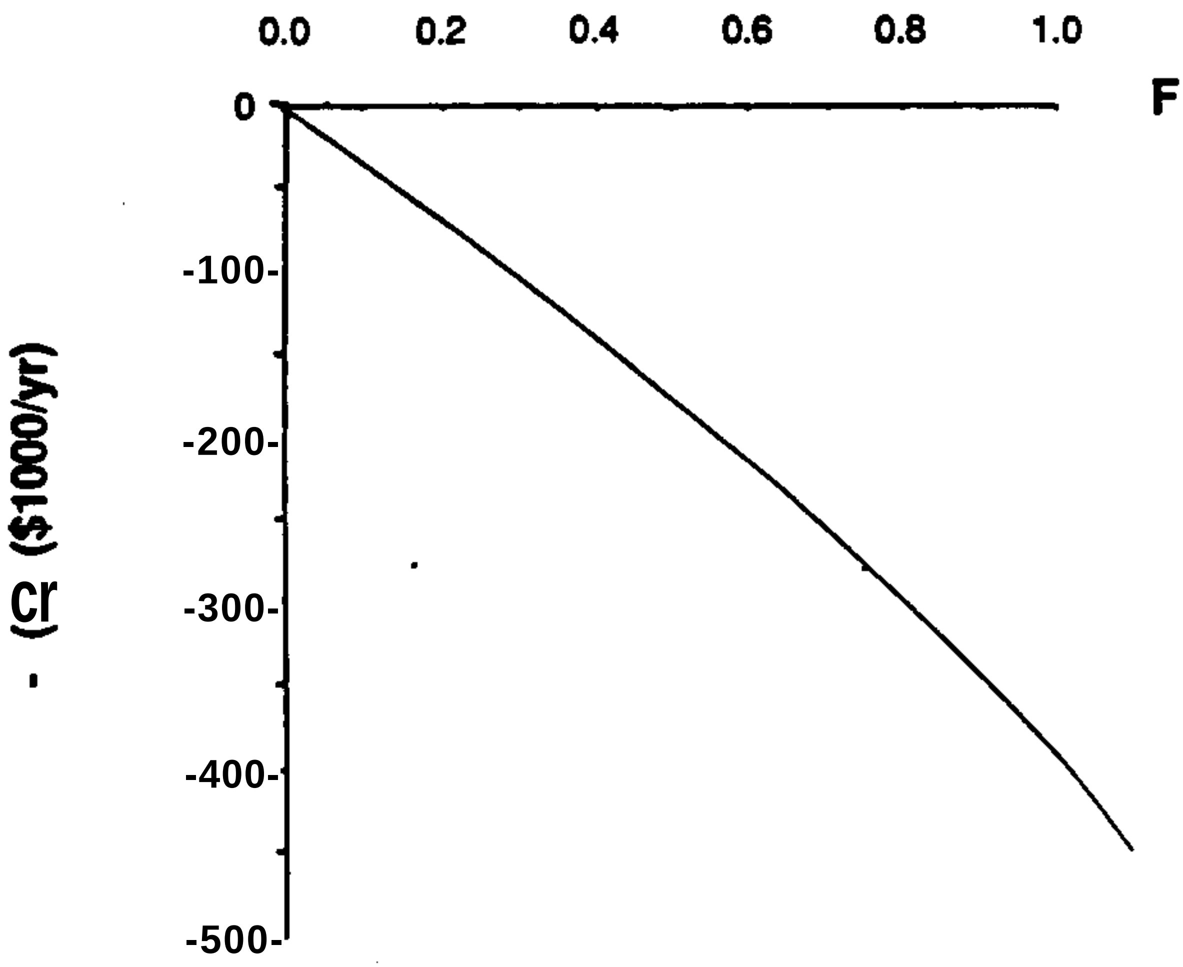

Fig. 8

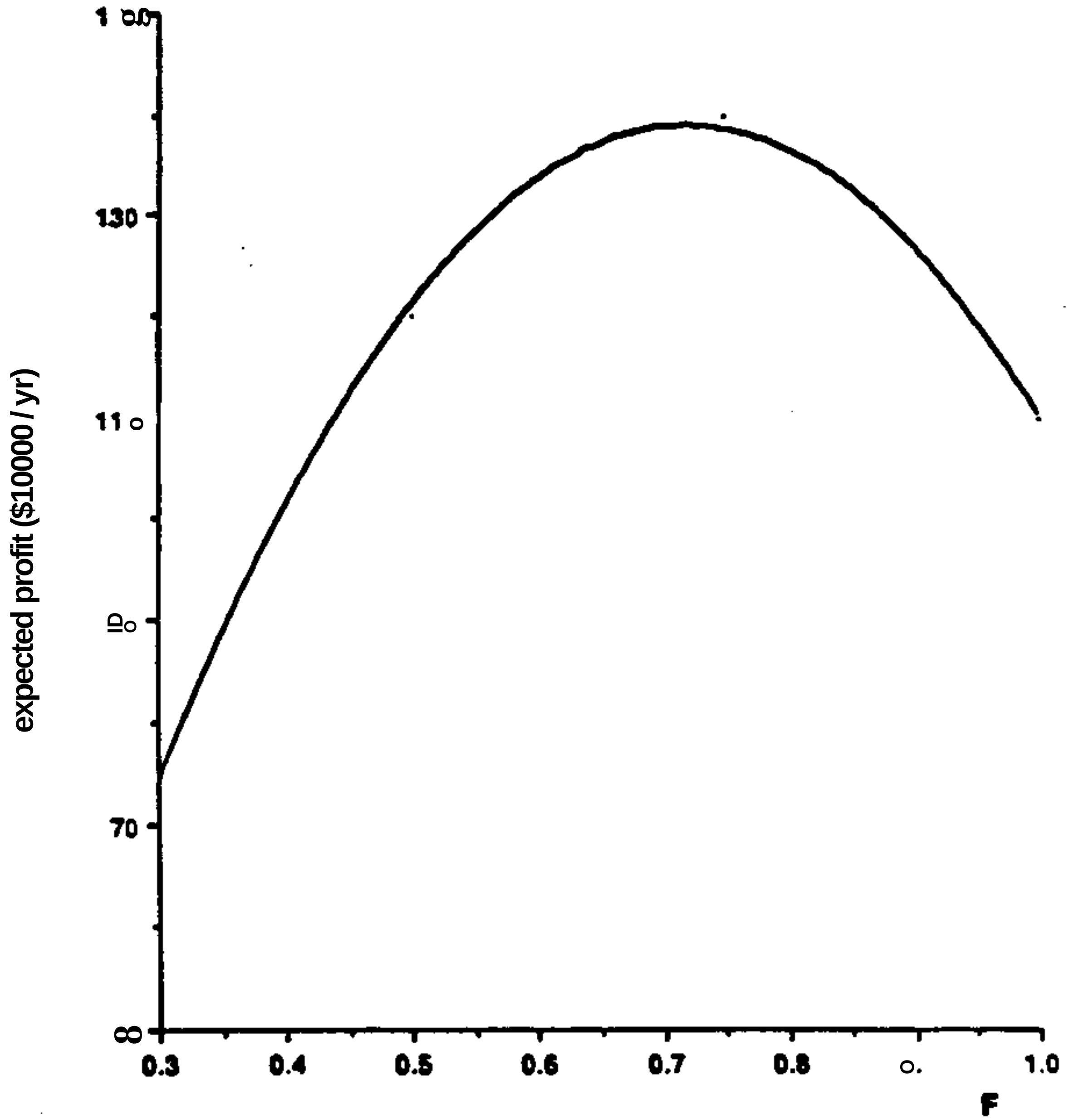

Fig. 9