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Optimum Design of Chemical Plants with Uncertain Parameters

A new strategy is proposed for the optimum design of chemical plants whose uncertain parameters are expressed as bounded variables. The design is such that the plant specifications will be met for any feasible values of the parameters while optimizing a weighted cost function which reflects the costs over the expected range of operation. The strategy is formulated as a nonlinear programme, and an efficient method of solution is derived for constraints which are monotonic with the parameters, a case which arises frequently in practice. The designs of a pipeline with a pump, of a reactor-separator system, and of a heat exchanger network, all with uncertain technical parameters, illustrate the effectiveness of the strategy for rational overdesign of a chemical plant.

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SCOPE

In the design of chemical plants, it is very often the case that some of the technical or commercial parameters are subject to significant uncertainty. In order to overcome this difficulty, the procedure which is normally used is to apply empirical overdesign factors to the sizes of the units. Other methods which predict more rational overdesign factors have been proposed, but their use in practice has been very limited. The main reasons for this is because the computational requirements of these methods are expensive and/or because the objectives in the basic strategy are not very realistic for design purposes. In this paper, a strategy is proposed which attempts to circumvent these difficulties. The objective of the proposed strategy is to design chemical plants which are able to meet the specifications for a bounded range of values of the parameters and which, at the same time, are optimum with respect to a weighted cost function. When probability distribution functions of the parameters are available, the expected value of the cost can be approximated by choosing appropriate weights. The mathematical formulation of the strategy leads to a large nonlinear program, where the inequality constraints must be maximized with respect to the uncertain parameters. The purpose of the paper is to derive a reasonable method of solution for the problem and to apply the strategy to typical design examples in chemical engineering, where uncertainty is present in parameters such as pump efficiencies, friction factors, reaction rate constants, and heat transfer coefficients.

CONCLUSIONS AND SIGNIFICANCE

An efficient method of solution for the nonlinear program is derived for the case where the constraints are monotonic with respect to the uncertain parameters, a case which arises frequently in practice owing to the sparsity of the constraints and to the monotonicity of the state variables with the technical parameters. The flexibility in the strategy lies in the fact that only bounds on the parameters are required, but that when probability distribution functions are available, the expected value of the cost can be estimated. The results of the examples show that the objectives of the strategy are quite suitable for design purposes and that the computational requirements are reasonable.

The optimum design of chemical plants operating at the steady state can be represented by the nonlinear program,

$$\min_{d,z} C(d, z, \theta)$$
$$\text{s.t. } h(d, z, \theta) = 0 \qquad (1)$$
$$g(d, z, \theta) \leq 0$$

Usually Equation (1) is solved for given nominal values of $\theta = \theta^N$, and empirical overdesign factors are applied to the optimum design variables to take into account the uncertainty in the parameters. Clearly, this procedure is not very satisfactory, and different methods have been proposed to evaluate the effect of the uncertainty in a more rational way.

Some methods take a statistical approach and assume that the probability distribution functions of the uncertain parameters are known (Kittrel and Watson, 1966; Wen and Chang, 1968; Weisman and Holzman, 1972; Watanabe et al., 1973; Lashmet and Szczepanski, 1974; Freeman and Gaddy, 1975; Johns et al., 1976; Paterson et al., 1977). Other methods take a deterministic approach (Takamatsu et al., 1973; Nishida et al., 1974; Dittmar and Hartmann, 1976; Kilikas, 1976) and assume that the uncertain parameters can be expressed as continuous and bounded variables

$$\theta^L \leq \theta \leq \theta^U \qquad (2)$$

where θ^L, θ^U, are specified bounds, which can also be interpreted as confidence limits for some unspecified distribution. In both approaches, the difference in the methods lies mainly in formulating the basic objectives, because the problem of optimum design with uncertain parameters is not well-defined.

In this paper, a new strategy is proposed for the optimum design of chemical plants when the uncertainty in the technical parameters is expressed as in (2). Its objective is to design plants that are always able to meet the specifications for any feasible values of the parameters and that, at the same time, are optimum with respect to a weighted cost function. This function can be used to estimate the expected value of the cost when probability distribution functions for the parameters are available.

STRATEGIES FOR BOUNDED PARAMETERS

One way of reformulating the nonlinear program in (1) when treating the parameters as in (2) is by solving the following problem as suggested by Nishida et al (1974):

$$\min_d \max_\theta C(d, z, \theta)$$
$$\text{s.t. } h(d, z, \theta) = 0 \qquad (3)$$
$$g(d, z, \theta) \leq 0$$
$$\theta^L \leq \theta \leq \theta^U$$

With this formulation, the plant is actually optimized at the value of the parameters that maximize the cost function. Although the solution of the minimax problem provides an upper bound for the cost, it does not ensure that the resulting design will fulfil the constraints

$$g(d, z, \theta) \leq 0 \qquad (4)$$

for arbitrary values of θ satisfying (2). An explicit way of achieving this has been suggested by Kwak and Haug (1976) when $C(d, z, \theta) = C(d)$ by solving the problem

$$\min C(d)$$
$$\text{s.t. } \max_{\theta^L \leq \theta \leq \theta^U} g_i(d, z, \theta) \leq 0 \quad i = 1, 2, \ldots s \qquad (5)$$
$$h(d, z, \theta) = 0$$

When $C = C(d, z, \theta)$, Takamatsu et al. (1973) have formulated a strategy in which Equation (1) is solved first for $\theta = \theta_N$, the nominal values. The cost function and the constraints are then linearized at the solution, and a linear program is then solved for the value $\theta = \theta^i$, which maximizes each component of (4). This value θ^i is chosen at one of the corner points of (2) using engineering judgment, and, of course, the method is only valid if such a value θ^i actually exists.

FORMULATION OF A NEW STRATEGY

The strategies presented in the last section tend to give very conservative results for chemical plants, as a unique value of d must be chosen. The fact is that after a plant has been built, the control variables can be adjusted in light of the actual conditions prevailing, and it may even be possible to modify the design. Thus, the vector d can be divided into two subsets of variables: the fixed design variables u which define the initially installed plant, and the control variables v which are chosen during operation and can therefore take account of the actual values of the parameters θ. For given u and θ, the control variables v will therefore be chosen to solve the problem

$$\min_{v,z} C(u, v, z, \theta)$$
$$\text{s.t. } g(u, v, z, \theta) \leq 0,$$
$$h(u, v, z, \theta) = 0, \qquad (6)$$

thus defining optimum values

$$v = \hat{v}(u, \theta), \quad z = \hat{z}(u, \theta),$$
$$\hat{C}(u, \theta) = C[u, \hat{v}(u, \theta), \hat{z}(u, \theta), \theta]$$

In fact, since v may include variables defining design modification or the portions of the plant actually in use, it may be necessary to add extra constraints to (1) to ensure that the installed capacity of the plant is not exceeded or to guarantee that the modified plant remains within its operability limits. Hence the new dimension t of the vector g of inequality constraint functions in (6) will, in general, be greater than s.

A first requirement of the initial design strategy is to choose the design variables u so that no matter what values of the parameters θ actually occur, it is possible to choose the control variables to meet the process objectives; in other words, to choose u so that (6) has feasible solutions for all θ satisfying (2). Within these limitations, it is desirable to choose u so that the average cost over the likely range of conditions is minimized, giving the formulation

$$\min_{u} E\{\hat{C}(u,\theta)\} \tag{7}$$

$$\text{s.t.} \max_{\theta^L \le \theta \le \theta^U} g_i[u, \hat{v}(u,\theta), \hat{z}(u,\theta), \theta] \le 0, \quad i = 1, 2, \ldots . t$$

Here the expected value of the cost is formally defined in terms of the parameter joint probability density $f(\theta)$

$$E\{\hat{C}(u,\theta)\} = \int_{\theta^{L_1}}^{\theta^{u_1}} \cdots \int_{\theta^{L_p}}^{\theta^{u_p}} \hat{C}(u,\theta) f(\theta) d\theta, \ldots \ldots d\theta_p \tag{8a}$$

but it will usually be adequate to approximate this integral by a finite weighted sum

$$E\{\hat{C}(u,\theta)\} \approx \sum_{j=1}^{n} \sigma_j \hat{C}(u,\theta^j) \tag{8b}$$

where the number of terms n and the weights σ_j, $j = 1, 2, \ldots . n$, should be chosen to fit the integral up to a certain order (see Gaussian and Radau integration formulas). However, the density function $f(\theta)$ will rarely be known sufficiently well to justify a high accuracy of fit, and it will usually be sufficient to select a relatively small number of points covering the likely range of the parameters and regard the σ_j as subjective probabilities for the sets θ^j, their choice being based simply on engineering judgment if no other information is to hand.

If (8b) is used in (7), we are concerned with only a finite number of parameter sets θ^j, $j = 1, 2, \ldots . n$, and a further simplification arises if the maximizing parameter sets θ^i, $i = 1, 2, \ldots . t$ for the constraints in (7) are taken as the first t sets θ^j, with $n \ge t$. We can then combine (6), (7), and (8b) and reformulate the problem as

$$\min_{u, v^j, z^j} \sum_{j=1}^{n} \sigma_j C(u, v^j, z^j, \theta^j)$$

$$\left.\begin{aligned} \text{s.t. } & g(u, v^j, z^j, \theta^j) \le 0 \\ & h(u, v^j, z^j, \theta^j) = 0 \end{aligned}\right\} j = 1, 2, \ldots . n$$

$$g_i(u, v^i, z^i, \theta^i) = \max_{\theta^L \le \theta \le \theta^U} g_i(u, v^i, z^i, \theta) \le 0,$$

$$i = 1, 2, \ldots \ldots . t. \tag{9}$$

If it is desired to specify the θ^j in the weighted objective function, for example to conform with a given integration formula, the formulation in (9) may still be used, simply setting $\sigma_j = 0$, $j = 1, 2, \ldots \ldots t$, with the remaining θ^j, $j = t + 1, \ldots n$ specified as required.

It is clear that at the solution of (9) we shall have $v^j = \hat{v}(u, \theta^j)$, $z^j = \hat{z}(u, \theta^j)$, solving (6) for each $j = 1, 2, \ldots . n$, and it is the inclusion of the constraints involving maximization that guarantees the operability of the plant within the constraints over the entire possible range of the parameters (even if they are allocated a zero weight, $\sigma_i = o$, in the objective function).

Equation (9) can be solved by standard nonlinear programming techniques, although in this general form it may well represent a formidable computing task, both because of the large number of constraints if n is large and because of the maximization subproblems in θ to be solved at each iteration of the variables u, v^j, z^j.

Special Solution for Monotonic Constraints

Because of the heavy computing requirements for the general problem, it is important to exploit any special structure in the equations for each particular design problem.

One special case, which results in substantial simplification, arises when the functions $g_i(u, v, z, \theta)$ are monotonic in each θ_k (with other variables fixed), for the maximization subproblems in (9) are then trivial. In fact, the solution of each subproblem must lie at a corner point of the polytope defined by (2), as is clearly seen from the relevant Kuhn-Tucker conditions:

$$-\frac{\partial g_i}{\partial \theta_k} = \lambda_k, \quad \lambda_k(\theta_k - \theta_k^L) \le 0, \quad \lambda_k(\theta_k - \theta_k^U) \le 0,$$

$$\text{for all } \quad k = 1, 2, \ldots . p, \quad i = 1, 2, \ldots . t \tag{10}$$

where if $\partial g_i/\partial \theta_k \ne 0$, $\theta_k^L \le \theta_k \le \theta_k^U$, we must have $\lambda_k \ne 0$ and hence either $\theta_k = \theta_k^L$ or $\theta_k = \theta_k^U$, depending on the sign.

Often, some or all of the equality constraints in (9) will be solved for the state variables z^j for each choice of u, v^j, θ^j (for example, using a flow sheeting package), rather than leaving these to be dealt with by the nonlinear programming algorithm. In this case, these equality constraints take the form $z = \Phi(u, v, \theta)$, and the above monotonicity property must then hold for the function $g_i(u, v, \Phi(u, v, \theta), \theta)$. The monotonicity property, in both of these forms, is surprisingly common, especially for technical parameters such as heat and mass transfer coefficients, reaction rate constants, and efficiencies, which derives from the fact that the constraints are sparse and the performance relations tend to be monotonic in these parameters. It is therefore worth examining the problem in some detail.

If the derivatives $\partial g_i/\partial \theta_k$ have the same sign for all feasible u, v, z, and θ (which is usually the case), the corner points θ^i, $i = 1, 2, \ldots . t$ can be determined once and for all, rather than at each iteration. Further, because of the sparsity, many constraints will be independent of particular parameters θ_k, making it possible to choose these arbitrarily in the θ^i and hence merge some of these sets to produce considerably fewer than t parameter sets to guarantee feasibility over the full range of parameter values. Finding μ, the minimum number of sets that contain all the active bounds, is a combinatorial problem whose solution can be determined efficiently using the algorithm described in the Appendix. In fact, the points where the merging takes place need not only be the corner points in (2), and other points can be considered as well. A suitable choice, as shown in the Appendix, is to consider points whose components can be any combination of lower, upper bounds, θ_i^L, θ_i^U, or additional points θ_i^j, $j = \mu + 1, \ldots . n$.

In order to determine the active bounds, the sign of the gradients of the constraints must be determined.

In practice, if the relevant derivatives are not easily determined, it may be simpler to assume monotonicity and use finite differences based on the nominal values and one limiting value for each parameter. This requires $(p + 1)$ process evaluations at any arbitrary value of d if the state variables are obtained in the form $z = \Phi(d, \theta)$. With the parameter values thus fixed, Equation (9) is reduced to solving

$$\min_{u,v^j,z^j} \sum_{j=1}^{n} \sigma_j C(u, v^j, z^j, \theta^j)$$

$$\left.\begin{array}{l} \text{s.t. } h(u, v^j, z^j, \theta^j) = 0 \\ \qquad g(u, v^j, z^j, \theta^j) \leq 0 \end{array}\right\} j = 1, 2, \ldots\ldots n \qquad (11)$$

where $n \geq \mu$, and θ^j, $j = 1, 2, \ldots\ldots n$ are chosen so as to guarantee feasibility of the constraints and to weight the objective function.

It is interesting to note that Equation (11) corresponds to a particular case of the nonlinear program formulated for the optimum design of multipurpose plants by Grossmann and Sargent (1977), so that their approach can be used to solve it.

It is usually desirable for the evaluation of the weighted cost function to include additional points beyond those strictly required to guarantee feasibility of the constraints. One obvious choice is to select the nominal value of the parameter θ^N, as this corresponds to the expected value of θ. Another reason is that the performance of chemical plants is usually specified at the nominal conditions of operation. When the probability distribution function $f(\theta)$ is available, the integral in (8) can be estimated as follows.

A grid is associated with the polytope in (2) by dividing each side $[\theta_k^L, \theta_k^U]$, $k = 1, 2, \ldots\ldots p$ into three equal intervals. This will then define 3^p elements of volume, V_i, $i = 1, 2 \ldots\ldots 3^p$. The μ points that guarantee feasibility will be contained in different elements V_i, and additional points to be considered should preferably also be located in different elements. If the distribution is symmetric, the volume in the center of the polytope will contain the nominal values. However, when the distribution is skewed, it is possible that a given element V_i contains the nominal values θ^N and one of the μ points. For such a case, or when, in general, a given element V_i contains more than one point, the procedure is to assign only one nonzero weight per element. The integral in (8) is then estimated by using n' of the 3^p elements V_i, $n' \leq n$, which contain at least one point, θ^j, $j = 1, 2, \ldots\ldots n$. When $n' \simeq 3^p$, the logical choice for the weights in (8b) is

$$\sigma_i = \phi_i \Big/ \sum_{j=1}^{n'} \phi_j \qquad (12a)$$

where

$$\phi_i = \int \ldots\ldots \int_{V_i} f(\theta) d\theta_1 \ldots\ldots d\theta_p \quad i = 1, 2, \ldots\ldots n'$$

However, when $n' << 3^p$, which, in fact, is the most frequent case, the use of (12a) can favor excessively the points of highest probability. To circumvent this, a heuristic choice of the weights is necessary, and the one which is recommended in this paper is to use

$$\sigma_i = \phi_i^{1/p} \Big/ \sum_{j=1}^{n'} \phi_j^{1/p} \qquad (12b)$$

When no distribution function is available, the weights must be specified by the designer. They can be chosen so as to reflect the subjective probability assigned by the designer to each one of the n conditions to be considered. Alternatively, zero weights can be assigned except for the nominal, worst, and best values of the parameters, the worst parameters being those which maximize the cost and the best parameters those which minimize it. However, in general, it is not a trivial problem to determine these parameters, since the former implies the solution of (3) and the latter the solution of a mini-min problem. Only when the cost is monotonic with the parameters and the same set of constraints remains active for any θ in (2) can the value of these parameters be determined easily.

DISCUSSION

The basic criterion of the proposed strategy, designing plants guaranteed to meet specifications under all conditions but which are optimal for the expected conditions, is clearly a desirable objective. However, since the formulation in (9) will, in general, require too much computational effort, examination of the validity of the assumptions implicit in the use of (11) will usually pay dividends.

The choice of the weights σ_j in the objective function can always be made heuristically and will not, in general, give rise to difficulties; the crucial assumptions are therefore the monotonicity of the inequality constraint functions. In some cases, it is possible to prove monotonicity when the constraints satisfy some sufficient conditions as shown by Grossmann (1977). For other cases, monotonicity can often be inferred from physical considerations. For example, it is known that product purities and recoveries vary monotonically with reflux or product rates in distillation columns, and the numerical examples give further instances. Often, preliminary examination of simplified models of units will provide the required information, and interactions through linked units in a process can be similarly checked. In practice, the monotonicity conditions can be expected to hold in a large number of cases, but for the exceptions it may still be possible to estimate the critical parameter values for which each constraint is maximized by engineering judgment or simplified analysis and, if necessary, allow a margin of safety in satisfying the inequalities for these values. Thus, the formulation in (11) is of much wider applicability than might at first appear.

NUMERICAL EXAMPLES

In order to illustrate the strategy, the following examples have been solved using the variable metric projection method of Sargent and Murtagh (1973) for solving the nonlinear program (11).

Pipeline with a Pump

The pipeline shown in Figure 1 must be designed in order to minimize the total annual cost

$$C = 196\,850\, D + 0.84632\, \hat{W}^{0.86} + 0.4251\, W \qquad (13)$$

It is assumed that there is uncertainty in the efficiency of the pump η and in the coefficient a of the friction

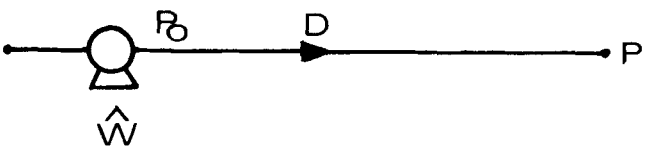

Fig. 1. Pipeline with a centrifuge pump.

TABLE 1. RESULTS FOR THE PIPELINE

			$\bar{C}$	$\hat{W}$	% overdesign	D	% overdesign
Nominal design			589 547	812 437	—	0.720641	—
σ_1	σ_2	σ_3					
0.8	0.1	0.1	667 662	1 370 140	68.6	0.757851	5.2
2/3	1/6	1/6	679 497	1 367 000	68.3	0.762506	5.8
1/3	1/3	1/3	708 950	1 359 960	67.4	0.773573	7.3
	Minimax		885 972	1 327 490	63.4	0.841103	16.7

factor $f = a/Re^{.16}$. Their nominal values are $\eta_N = 0.5$ and $a_N = 0.04$, and their bounds are

$$0.3 \leq \eta \leq 0.6, \quad 0.02 \leq a \leq 0.06 \tag{14}$$

The required power of the pump is given by

$$W = \frac{994.018}{\eta}\left[\frac{P - 101\,352.928}{2\,394.012} + \frac{5.6608566\,a}{0.04\,D^{4.84}}\right] \tag{15}$$

and must not exceed the installed power of the pump

$$\hat{W} \geq W \tag{16}$$

The outlet pressure $P(N/m^2)$ must satisfy the constraint

$$1\,013\,529.28 - P \leq 0 \tag{17}$$

Clearly, for the pump $\partial P_o/\partial\eta > 0$, where P_o is the outlet pressure of the pump, for the pipeline $\partial P/\partial P_o > 0$, and $\partial P/\partial a < 0$. It then follows that for any value of $\hat{W}$, D, and W, Equation (17) is maximized at η_L, a_U.

It can easily be proved that Equation (17) will be active for any value of the parameters. This can then be used to establish that the value of the parameters which maximize the cost are η_L and a_U and the ones that minimize the cost are η_U and a_L. These will then define the best and the worst parameters. As the nominal values of the parameters are considered for weighting the cost function, the problem to be solved according to (11) is

$$\min \bar{C} = 196\,850\,D + 0.84632\,\hat{W}^{0.86} + 0.4251\sum_{i=1}^{3}\sigma_i W_i$$

$$\text{s.t.} \quad W_i = \frac{994.018}{\eta^i}\left[381.024135 + \frac{5.6608566\,a^i}{0.04\,D^{4.84}}\right]$$

$$\hat{W} \geq W_i \quad i = 1, 2, 3 \tag{18}$$

$$0.508 \leq D \leq 0.9144$$

$$\eta^1 = 0.5 \quad \eta^2 = 0.3 \quad \eta^3 = 0.6$$

$$a^1 = 0.04 \quad a^2 = 0.06 \quad a^3 = 0.02$$

The problem was solved for three different sets of weighting factors, and in order to obtain the overdesign factors, the nominal design was determined. The overdesign factors were defined as

$$\text{odf} = (d_o - d_N)/d_N \tag{19}$$

The results are shown in Table 1, where it can be seen that the overdesign factors are not very sensitive to the three sets of weights. With the minimax strategy, which in this particular case corresponds to solving (18) with $\sigma_1 = 0$, $\sigma_2 = 1$, $\sigma_3 = 0$, the overdesign factors were significantly different from the others.

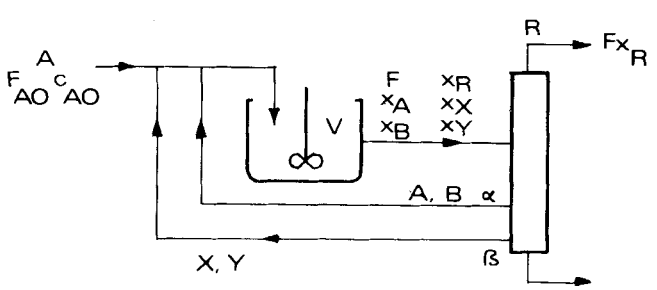

Fig. 2. Reactor-separator system.

Reactor-Separator System

This problem has been taken from Takamatsu et al. (1973). The system shown in Figure 2 consists of a CSTR of volume V (m^3) with perfect mixing, and it is assumed that Denbigh's reaction takes place with first-order irreversible kinetics

$$\begin{array}{ccccc} & & k_B & k_R & \\ A & \rightarrow & B & \rightarrow & R \\ & & \downarrow k_X & \downarrow k_Y & \\ & & X & Y & \end{array} \tag{20}$$

The outlet flow of the CSTR is F, whose molar concentrations of the five components are x_A, x_B, x_R, x_X, x_Y.

It is assumed that the separator produces a perfect split obtaining only product R at the top. At the bottom, fraction α of components A and B and fraction β of components X and Y are recycled in order to be mixed with an inlet stream of pure A whose flow and concentration is F_{AO} and c_{AO}. For the steady state and isothermal operation, the process can be described for the different operating conditions $k = 1, 2, \ldots n$ with the following system of nonlinear equations:

$$\begin{aligned}
&F_{AO} - x_A{}^k F^k(1-\alpha^k) - V(k_B + k_X)c_{AO}x_A{}^k = 0\\
&-F^k x_B{}^k(1-\alpha^k) + Vc_{AO}[k_B x_A{}^k - (k_R + k_X)x_B{}^k] = 0\\
&-F^k x_X{}^k(1-\beta^k) + Vc_{AO}k_X x_A{}^k = 0\\
&-F^k x_Y{}^k(1-\beta^k) + Vc_{AO}k_Y x_B{}^k = 0\\
&-Fx_R{}^k + Vc_{AO}k_R x_B{}^k = 0\\
&x_A{}^k + x_B{}^k + x_R{}^k + x_X{}^k + x_Y{}^k - 1 = 0 \quad k = 1, 2, \ldots n
\end{aligned} \tag{21}$$

The minimum amount of R that has to be produced is F_R, yielding

$$F_R - F^k x_R{}^k \leq 0 \quad k = 1, 2, \ldots n \tag{22}$$

The nominal values of the rate constants and other parameters are given in Table 2.

TABLE 2. DATA FOR THE REACTOR-SEPARATOR SYSTEM

$k_B = 0.4\,h^{-1}$ $k_R = 0.1\,h^{-1}$ $k_X = 0.02\,h^{-1}$ $k_Y = 0.01\,h^{-1}$
$F_{AO} = 100$ mole/h $c_{AO} = 100$ mole/m^3 $F_R = 70$ mole/h
$c_1 = \$10/m^3$ $c_2 = \$0.125$/mole

Table 3. Results for the Reactor-Separator System

σ_1	σ_2	σ_3	$\bar{C}$	V	% overdesign
Nominal design			151.92	12.3466	—
2/3	1/6	1/6	160.7	13.3962	8.3
1/3	1/3	1/3	165.7	13.8735	12.2
	Minimax		185.66	15.5854	26.0

If we assume that the rate constants have an uncertainty of ±20% with respect to their nominal values, they will be bounded as follows:

$$\begin{aligned} 0.32 \leq k_B \leq 0.48 \\ 0.08 \leq k_R \leq 0.12 \\ 0.016 \leq k_X \leq 0.024 \\ 0.008 \leq k_Y \leq 0.012 \end{aligned} \tag{23}$$

The total cost of the system is given by

$$\bar{C} = c_1 V + c_2 \sum_{k=1}^{n} \sigma_k [\alpha^k F^k (x_A{}^k + x_B{}^k) + \beta^k F^k (x_X{}^k + x_Y{}^k)] \tag{24}$$

where the first term represents the cost of the reactor and the second term the cost of the recycle.

Calculating numerically the gradient of (22), we found that (22) is maximized at k_{BL}, k_{RL}, k_{XU}, k_{YU} which is what we expected from the physics of the process. Here it is not obvious that the cost will be monotonic with the rate constants, keeping constraint (22) active. As a result of this, and in order to have an appropriate weighting of $\bar{C}$, apart from the nominal values, a third value for the parameters was taken at the opposite bounds of the ones that maximize (22), k_{BU}, k_{RU}, k_{XL}, k_{YL}. The weight σ_1 was assigned to the nominal values and σ_2, σ_3 to the two other values. The problem is then to choose V, α^k, β^k, $k = 1, 2, 3$ in order to minimize (24) subject to constraints (21) and (22) for the three values of the parameters described above.

The problem was solved for two different sets of weights, for only the nominal parameters, and for the parameters at k_{BL}, k_{RL}, k_{XU}, k_{YU}, which most probably correspond to the solution of the minimax problem, although no attempt was made to check this. The results are shown in Table 3, where it can be seen that the overdesign factors with the proposed strategy are much smaller than the one obtained with the minimax strategy. It is to be noted that constraint (22) was active in all the cases.

Heat Exchanger Network

The network to be optimized corresponds to the optimal network 4SP1 in Lee et al. (1970), where the data and specifications can be found. The network is shown in Figure 3. The outlet temperatures T_3, T_6, T_{10}, T_{12}, T_{15} were specified as inequalities, and the steam

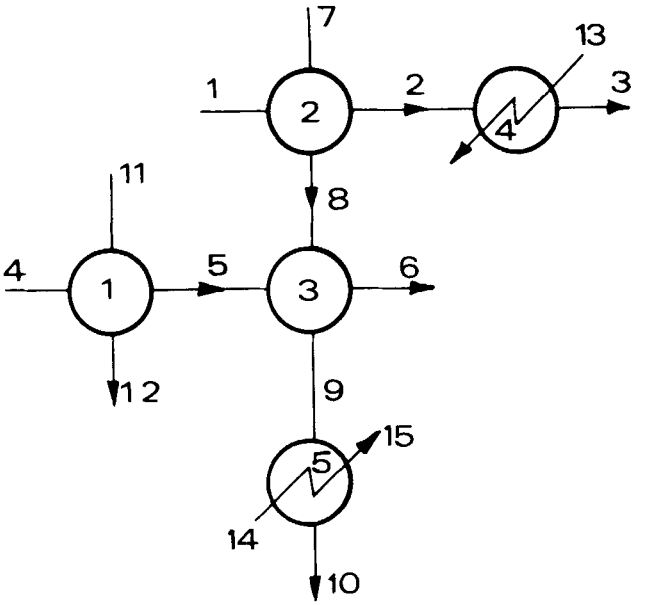

Fig. 3. Heat exchanger network.

Table 4. Active Bounds of the Set of Constraints (27)

Constraints	Active bounds for nonzero gradients
1	U_{L2}, U_{L4}
2	U_{L1}
3	U_{L1}, U_{U2}, U_{L3}
4	U_{U1}, U_{L2}, U_{L3}, U_{L5}
5	U_{U1}, U_{U2}
6	U_{U2}, U_{U4}
7	U_{U1}
8	U_{U2}
9	U_{U1}, U_{U2}, U_{U3}
10	U_{L1}, U_{U2}, U_{U3}

temperature T_S was controlled with a valve. This was done in order to introduce enough degrees of freedom in (11) as suggested by Grossmann and Sargent (1977).

It was also assumed that the latent heat of the steam was given by

$$\lambda = -19.78211\, T_S{}^2 + 15\,535.673\, T_S - 999\,269.2 \tag{25}$$

where λ is given in Joules per kilogram, and T_S is the steam temperature such that $T_S \leq 555.3722$°K.

A ±20% uncertainty in the value of all the heat transfer coefficients U_i, $i = 1, 2, \ldots 5$, was considered. The problem is then to choose the areas A_i, $i = 1, 2, \ldots 5$, (m^2) the steam temperatures $T_S{}^k$, $k = 1, 2, \ldots n$ and the outlet temperatures of the cooling water $T_{WO}{}^k$, $k = 1, 2, \ldots n$ in order to minimize the total annual cost

$$\bar{C} = \sum_{i=1}^{5} c_o A_i{}^\beta + \sum_{k=1}^{n} \sigma^k (c_S F_S{}^k + c_W F_W{}^k) \tag{26}$$

where $F_S{}^k$, $F_W{}^k$, $k = 1, 2, \ldots n$, are the steam and cool-

Table 5. Results for the Heat Exchanger Network

σ_1	σ_2	σ_3	σ_4	σ_5	$\bar{C}$	A_1	A_2	A_3	A_4	A_5
Nominal design					9 959.7	24.659	70.446	40.637	3.602	1.735
0.6	0.1	0.1	0.1	0.1	11 757.8	30.823	65.019	45.576	3.904	2.849
% overdesign					—	25	−7.7	12.2	8.4	64.2

ing water flow rates, and c_o, β, c_S, c_W are cost parameters whose values are given in Lee et al. (1970). The constraints are given by the heat balances and by the following inequalities:

$$\begin{aligned} T_3^* - T_3^k &\leq 0 \\ T_{12}^k - T_{12}^* &\leq 0 \\ T_6^* - T_6^k &\leq 0 \\ T_{10}^k - T_{10}^* &\leq 0 \\ T_5^k - T_8^k &\leq 0 \end{aligned} \qquad k = 1, 2, \ldots n \quad (27)$$

$$\begin{aligned} \delta - T_3^k + T_{13}^k &\leq 0 \\ \delta - T_{11}^k + T_5^k &\leq 0 \\ \delta - T_7^k + T_2^k &\leq 0 \\ \delta - T_8^k + T_6^k &\leq 0 \\ \delta - T_9^k + T_{15}^k &\leq 0 \end{aligned}$$

T_i^*, $i = 3, 6, 10, 12$, denote the specified outlet temperatures. Unlike Lee et al. (1970), the value of δ was taken as 5/9°K.

The signs of the gradients of the constraints in (27) were determined by using finite differences to determine the bounds of the heat transfer coefficients which are active when the constraints in (27) are maximized, and they are shown in Table 4.

Merging all the active bounds by the procedure described in the Appendix, four minimum points were found: $U^2 = (U_{U1}, U_{U2}, U_{U3}, U_{U4}, U_{N5})$, $U^3 = (U_{L1}, U_{U2}, U_{U3}, U_{U4}, U_{N5})$, $U^4 = (U_{U1}, U_{L2}, U_{L3}, U_{L4}, U_{L5})$, $U^5 = (U_{L1}, U_{U2}, U_{L3}, U_{U4}, U_{N5})$. The weights σ_2, σ_3, σ_4, σ_5, were assigned to these points and the weight σ_1 to the nominal value of the parameters, $U^1 = (U_{N1}, U_{N2}, U_{N3}, U_{N4}, U_{N5})$. The problem was solved for one set of values for the weights, and also the nominal design was determined. The results are shown in Table 5.

It is interesting to note that the second area has a negative overdesign factor. This was because the eighth constraint in (27) was active at the solution when $U_2 = U_{U2}$. This means that if a larger area were used in exchanger 2, the temperature approach would be less than δ for $U_2 = U_{U2}$, as the heat flow rate of hot stream 1 is smaller than the heat flow rate of cold stream 7. Finally, only the temperature of stream 3 was at its specified outlet temperature for the five values of the parameters, whereas the temperature of stream 6 was always above its specified outlet temperature.

CONCLUSIONS

The objectives of the strategy which has been proposed seem to be quite appropriate for the design of chemical plants with uncertain parameters. The simplified method of solution which has been derived for monotonic inequality constraints can be applied for a very large number of practical cases. The three numerical examples which have been solved show that the proposed strategy provides a rational and economical way of obtaining safe optimum designs when the specifications or data are subject to uncertainty.

NOTATION

A = raw material (reactor example)
$A(\mathrm{m}^2)$ = heat exchange area
$A = [a_{ij}]$ = matrix of active bounds
$a(-)$ = coefficient in friction factor formula
B = matrix derived from A by deleting rows
C = cost function
$\hat{C}, \hat{v}, \hat{z}$ = optimum values of C, v, z, respectively
$C^k = \{c_1, \cdots c_p\}$ = set of corner points of (2)
$c_{Ao}(\mathrm{mole/m}^3)$ = feed concentration (of A)
c_o, c_s, c_w = cost coefficients
$c_1(\$/\mathrm{m}^3)$, $c_2(\$/\mathrm{mole})$ = cost coefficients
d = m vector of design and control variables
d_N = size determined in nominal design
d_o = size determined with strategy
$D(\mathrm{m})$ = pipe diameter
$E\{\cdot\}$ = expectation operator [with respect to distribution $f(\theta)$]
$f(\theta)$ = parameter joint probability density
$f(-)$ = friction factor
$F, F_R(\mathrm{mole/h})$ = actual and minimal production rate
$F_{Ao}(\mathrm{mole/h})$ = feed rate
F_s, F_{cw} = steam and cooling water flow rates
g = s vector or t vector of inequality constraint functions
h = r vector of equality constraint functions
$I = \{1, 2, \cdots t\}$ = index set of constraints
i, j = running indexes
i, j, r, s = row and column labels
$J = \{1, 2, \cdots p\}$ = index set of parameters
K = index set of corners
$|K|$ = number of elements in K
k, l = set element labels
$k_B, k_R, k_X, k_Y(\mathrm{h}^{-1})$ = reaction rate constants
L, Q, R, S, T = index sets used in algorithm (Appendix)
m = dimension of vector d
n = number of terms in weighted objective function
n' = number of volume elements V_i
odf = overdesign function
p = dimension of vector θ
$P(\mathrm{N/m}^2)$ = outlet pressure
$P_o(\mathrm{N/m}^2)$ = pump delivery pressure
r = dimension of vector h
R = desired product
Re = Reynolds Number
s, t = dimension of vector g
T_i = temperature of stream i
T_s = steam temperature
T_{WO} = cooling water outlet temperature
T_i^* = minimum temperature of stream i
u = vector of fixed design variables
U_i = heat transfer coefficient for exchanger
u, w, x, γ, Ω = weights used in algorithm (Appendix)
v = vector of control variables
$V(\mathrm{m}^3)$ = reactor volume
V_i = elements of volume in estimating the objective function
$W, \hat{W}$ = Watt actual and installed power of pump
$x_A, x_B, x_R, x_X, x_Y(\mathrm{mole/m}^3)$ = molar concentrations of A, B, R, X, Y, respectively
X, Y = undesirable by-products
z = r vector of state variables

Greek Letters

$\alpha(-)$ = recycle ratio of A and B
β = cost index
$\beta(-)$ = recycle ratio of X and Y
δ = minimum temperature approach
$\eta(-)$ = pump efficiency
θ = p vector of parameters
$\theta^N, \theta^L, \theta^U$ = nominal value, lower and upper bounds for θ
λ = Kuhn-Tucker multiplier, latent heat of steam
μ = minimum number of points to guarantee feasibility
σ_j = weights in objective function
Φ = equality constraint function

ϕ = empty set
ϕ_i = integral of $f(\theta)$ over V_i

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APPENDIX: ALGORITHM FOR MERGING THE ACTIVE BOUNDS IN THE MINIMUM NUMBER OF POINTS

The active bounds for the maximization of the constraints in (9) can be represented by matrix A, $A = [a_{ij}]$, where

$$a_{ij} = \begin{cases} 0 \text{ if } \partial g_i/\partial\theta_j = 0 \\ 1 \text{ if } \theta_j^L \text{ is active, that is } \partial g_i/\partial\theta_j < 0 \\ 2 \text{ if } \theta_j^U \text{ is active, that is, } \partial g_i/\partial\theta_j > 0 \end{cases} \qquad (A1)$$

$$i \in I = \{1, 2, \ldots t\} \quad j \in J = \{1, 2, \ldots p\}$$

Any corner point in (2) will be represented by the ordered set

$$C^k = \{c_1, c_2, \ldots c_p\}$$

where $c_j = 1$ or 2, $j \in J$, and $k \in K$, where K is the index set of all the corners. If $|K|$ is the number of elements in set K, it is clear that $|K| = 2^p$.

The problem of finding the minimum number of corner points that contain all the active bounds can then be formulated as follows: given matrix A and the set K, determine a subset K', $K' \subseteq K$, for which $|K'|$ is a minimum, μ, and for which a subset I^k exists, $I^k \subseteq I$, for each k in K', so that $a_{ij} = c_j$ in C^k for all $j \in J$ when $a_{ij} \neq 0$, $i \in I^k$. The following algorithm is proposed for solving this problem:

Step 1—(a) determine the set $S^o = \{k | a_{ik} = 0 \text{ or } 1 \text{ for all } i \in I, \text{ or } a_{ik} = 0 \text{ or } 2 \text{ for all } i \in I\}$. ($b$) define $c_k' = \max_{i \in I} \{a_{ik}\}$, $k \in S^o$. (c) If $S^o = J$, the solution is $\mu = 1$ with the corner $C' = \{c_1', c_2', \ldots c_p'\}$.

Step 2—define matrix $B = [b_{ij}]$, by eliminating row r in A if row s, $s \neq r$, exists in A, such that $a_{rj} \neq a_{sj}$ implies $a_{rj} = 0$, $j \in J^1$ and $a_{rj} = a_{sj}$, $j \in J^2$, where $J^1 \cup J^2 = J$, $J^1 \cap J^2 = \phi$. Define I_B, $I_B \subseteq I$, the index set of rows in B.

Step 3—(a) set $Q = \phi$, $T = L$, where $L = \{l\}$ is the index set of the subset of corners $C^l = \{c_1, c_2, \ldots c_p\}$ such that $c_j \neq c_j'$, $j \in S^o$, $c_j = 1$ or 2, $j \notin S^o$, $j \in J$. (b) generate one corner $C^k = \{c_1, c_2, \ldots c_p\}$ where $k \in T$, $c_j = 1$ or 2, $j \in S^o$, $c_j = c_j'$, $j \in S^o$, $j \in J$. Include k in T. (c) determine $S^k = \{i | i \in I_B, b_{ij} = c_j \text{ for all } j \in J \text{ when } b_{ij} \neq 0\}$. If $S^k \neq \phi$, include k in Q. If $|Q| \leq 1$ go to (e). (d) calculate $R = S^k \cup S^l$, $k, l \in Q$, $k \neq l$. If $R = S^k$, exclude l from Q. If $R = S^l$, exclude k from Q. (e) if $|T| < |K|$, go to (b).

Step 4—(a) calculate $\gamma = \max \{2, \Omega\}$ where $\Omega = \sum_{l \in Q} w_l$ and

$$w_l = \begin{cases} 1 \text{ if } \bigcup_{k \in Q} S^k - \bigcup_{\substack{k \in Q \\ k \neq l}} S^k \neq \phi \\ 0 \text{ otherwise} \end{cases} \qquad (A2)$$

If $\gamma = |Q|$, the solution is $\mu = \gamma$ with the corners C^k, $k \in Q$. (b) solve the set covering problem

$$\min \sum_{q \in Q} x_q \qquad (A3)$$

$$\text{s.t.} \quad \sum_{q \in Q} u_{iq} x_q \geq 1 \qquad i \in I_B$$

$$x_q = 0,1 \quad q \in Q$$

where x_q is associated with the existence of corner q in the set K' and

$$u_{iq} = \begin{cases} 1 \text{ if } b_{ij} = c_j \text{ in } C^q \text{ for all } j \in J \text{ when } b_{ij} \neq 0 \\ 0 \text{ otherwise} \end{cases} \qquad (A4)$$

The solution is then $\mu = \sum_{q \in Q} x_q$ with the corners C^k, $k \in K' = \{q | x_q = 1\}$. Problem (A3) can be solved with an implicit enumeration algorithm as proposed in Garfinkel and Nemhauser (1972).

It should be noted that the efficiency of the algorithm of this Appendix stems from the following facts:

1. $|K - L|$ corner points are enumerated from the $|K|$ possible enumerations.
2. No more than $|Q|$ corner points need to be stored.
3. The size of problem (A3) is reduced effectively as it involves $|Q|$ variables, $|Q| \leq |K|$, and $|I_B|$ constraints, $|I_B| \leq |I|$.

Since, in general, K' is not unique for the same μ, the weighted cost function in (11) will be affected by taking different corner points. This difficulty can be circumvented to some extent by defining for each corner $C^k = \{c_1, c_2 \ldots c_p\}$, $k \in K'$, $c_j = 3$ when $a_{ij} = 0$ for all $i \in I^k$, where 3 is associated with the nominal value of the parameters θ^N or, more generally, any of the additional points $\theta^j = \mu + 1, \ldots n$. In this way, the multiplicity of the solutions can be considerably reduced.

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