neering, 11, 392 (1966).
———, "Vapor Liquid Equilibria, Correlation by Means of Modified Redlich Kwong Equation of State," *ibid.*, 9, 168 (1964).
Woods, D. R., T. W. Hoffmann, and A. I. Johnson, "Teaching Experience with Design and Simulation Project," *Chem. Eng. Educ.*, 7(2), 96 (1973).
Worley, F. L., Jr., and R. L. Motard, "Information Systems in Chemical Engineering Design," Chem. Eng. Computation, Vol. 2, AIChE Workshop Series (1972).

THE AUTHORS

Rodolphe L. Motard received his B.S. in chemical engineering from Queen's University, Canada, and his M.S. and D.Sc. in chemical engineering from Carnegie Mellon University. From 1951-1957 he worked for Shell Oil Company and subsequently joined the faculty of the University of Houston, where he is Professor of Chemical Engineering and Director, Systems Simulation Laboratory. He is spending the 1974-1975 academic year at the Computer Aided Design Centre, Cambridge, England.

Mordecai Shacham received his B.Sc. and D.Sc. in chemical engineering from the Technion, Israel Institute of Technology. He spent the 1973-1974 academic year on a post-doctorate fellowship at the University of Houston and is currently with Ben-Gurion University, Beersheva, Israel.

Edward M. Rosen received his B.S. and M.S. degrees from the Illinois Institute of Technology and his Ph.D. from the University of Illinois. Currently he is a Science Fellow and Manager, Systems Technology at the Monsanto Company where he has been since 1959, except for a postdoctoral academic leave at Stanford University in 1962-1963. With E. J. Henley, he is co-author of the text *Material and Energy Balance Computations* (1969). His hobbies include violin and foreign language study.

Quantitative Overdesign of Chemical Processes

Overdesign is applied to chemical processes to account for expected variations in the design data or design conditions. These variables must be treated quantitatively in order to design a process that is certain to perform adequately. Process dependability is introduced as a means of quantifying variable process behavior. Overdesign using the dependability criterion is a stochastic optimization problem. An example problem with three stochastic variables and two design variables is presented to illustrate these procedures.

R. A. FREEMAN
Monsanto Company
St. Louis, Missouri 63166
and
J. L. GADDY
Department of Chemical Engineering
University of Missouri
Rolla, Missouri 65401

SCOPE

In recent years, developments such as sophisticated optimization methods and process synthesis techniques have significantly advanced the procedures of process design. However, the final stage of design, that of specification of overdesign or safety factors, is still largely a subjective procedure based upon experience.

In general, safety factors are increased as the uncertainty of the process variables increases; a procedure that can be expensive if safety factors are specified too small or too large. Recent studies to quantify overdesign represent the uncertain parameters as random variables and compute the overdesign based upon the expected value criterion.

The expected value is not always suitable for evaluating chemical processes since adverse deviations from the average might mean unacceptable or even hazardous performance. Also, these methods have only been applied to a few processes where the statistical behavior of a process performance criterion is known or can be obtained analytically.

The purpose of this study is to demonstrate how overdesign can be achieved by the use of a process dependability criterion and stochastic simulation procedures. A simple process involving a reactor and separator was chosen for study. This process has both variable conditions and uncertain data, with two design variables, reactor volume and number of separator stages.

CONCLUSIONS AND SIGNIFICANCE

The use of process dependability, the fraction of time the process must meet certain performance criteria, was found to be an improved method of designing and optimizing a chemical process. Since there are many combinations of the design variables that produce the same process dependability, the selection of the proper design becomes an optimization problem. An exhaustive search procedure was applied to the solution of this stochastic optimization problem.

The optimum design of this process was found to be surprisingly different from the design based upon the usual methods. An overdesign factor of 350% is optimal for the reactor while less than 10% is required for the column.

Uncertainty in process design can be of two types: doubtful design data or variable design conditions. Known or suspected errors in the design data or computational procedures introduce uncertainty into the final design. Also, fluctuations in design conditions, pressure, temperature, flow, etc., that are uncontrollable may cause the performance of the design to be inadequate. Most design procedures use the average value of the uncertain parameters in the design model. When a parameter deviates from the average, the process may not perform as designed unless an adequate overdesign factor has been used.

Analytical methods of overdesign represent the variables in the design model as random variables and use statistical procedures to predict a reliable design. One such approach, based on variance analysis techniques, has found use in the study of mechanical systems (Mischke, 1970; Svenson, 1961; Su, 1960). In the design of chemical systems, most investigations (Chen et al., 1970; Kitrell and Watson, 1966; Saletan and Caselli, 1963) have been based upon the expected value criterion.

These methods permit calculation of the probability of failure or the expected value of the performance of a given design, provided some knowledge of the statistics of a process performance criterion is available. These data may be obtained analytically for simple process models with a few random variables. However, for more complex processes, these methods cannot be used unless simplifying assumptions are made. Furthermore, there is the restriction that the expected value be a representative criterion for judging process performance. More recent studies (Freeman and Gaddy, 1973; Lashmet and Szczepanski, 1974; Berryman and Himmelblau, 1973) have used numerical methods to obtain the probability of process performance.

DEPENDABILITY AS AN OVERDESIGN CRITERION

For a chemical process with variable, perhaps random, design data or design conditions, it is recognized that the process performance will also be variable. Unless the design is based upon the worst possible conditions, the process will not always perform satisfactorily, that is, produce a product that meets specifications. The question of overdesign can then be related to determining the fraction of time the process must perform to meet certain criteria. This fraction of acceptable performance defined by Equation (1) is named dependability (Freeman and Gaddy, 1973), and offers a means of quantifying the uncertainty of variable process behavior:

$$D = \int_{-\infty}^{l} f(x)\, dx \tag{1}$$

Equation (1) is simply the expression for the cumulative probability of a process performance criterion, such as product concentration x. If the variables in the system are time variables, the dependability is the fraction of time the process must meet a performance limit, such as producing product meeting a minimum concentration specification, l.

It should be noted that dependability is different from process reliability (Ufford, 1972; Coulter and Morello, 1972), the term generally applied to define the percentage of time the process will not fail due to equipment malfunction or breakdown. Dependability defines the percentage of time the process fails whether operating or not and can include equipment breakdown.

The design of a process using the dependability criterion requires the probability density function $f(x)$ of the process performance measure. Since this function will probably be unknown and difficult to obtain analytically, it can be found numerically by stochastic (Monte Carlo) simulation. This procedure (Tayyabkhan and Richardson, 1965; Hess and Quigley, 1963; Gaddy and Culberson, 1973) requires that the variables in the process be represented as random variables.

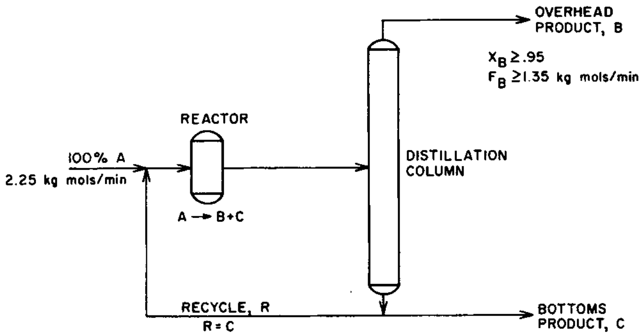

Fig. 1. Process flow diagram.

The procedure of design using the dependability criterion will be demonstrated with an example. The example process chosen has three random variables, including both uncertain data and variable design conditions.

DESIGN BY STOCHASTIC SIMULATION

Consider the problem of designing the simple chemical process shown in Figure 1. A first-order reaction decomposes raw material A into product B and waste material C. The reaction products are separated in a distillation column and half of the bottoms stream, containing A and C, is recycled back to the reactor.

The design variables in this process are the reactor volume and the number of stages in the column. The design equations for sizing the reactor and column are given in Table 1. Equation (2) permits calculation of the reactor effluent concentration from the reaction rate constant, inlet flow and composition, and reactor volume. This equation assumes ideal mixing and no volume change upon reaction. Equation (3) (Gilliland, 1940) allows estimation of the column stages from the minimum stages, Equation (4) (Fenske, 1932), and the minimum reflux ratio, Equation (5) (Underwood, 1946).

Design of this process is straightforward provided the inlet and outlet conditions are fixed and the design data are available. However, in this example, the design conditions and data are variable, as shown in Table 2; (1) the flow rate of raw material is variable, (2) the reaction rate constant is uncertain, and (3) the column reflux ratio can be controlled only within certain limits. These variations were considered random, with triangular probability distributions (Sprow, 1967; Gaddy and Culberson, 1973) defined by the minimum, maximum, and most likely values of each variable.

The product specifications require that the flow rate be at least 1.35 kg mols/min. with a composition of 95% or better. With these dual specifications, the dependability is defined by a bivariate density function:

$$D = \int_{-\infty}^{.95} \int_{-\infty}^{1.35} g(x_B, B)\, dx_B dB \tag{6}$$

The dependability can be found by stochastic simulation and the function $g(x_B, B)$ does not need to be known explicitly. In this example, the dependability represents the fraction of the time the process must produce product to meet both specifications.

Dependability, alone, may not be sufficient as a design criterion. If the process must always meet specifications, that is, $D = 1$, the design would be based upon the most adverse values of Q, k, and L/D. These conditions would require the maximum overdesign of volume and number of stages, and this design may be too costly. Therefore, the choice of the level of dependability should be an economic balance between the cost of overdesign and the cost of off-spec product.

In this process, as the reactor volume is increased, the concentration of B in the reactor effluent increases. Consequently, the tower size to produce a given product purity can be smaller. Thus, there are many combinations of volume and stages that will yield the same dependability; and, the choice of these variables must also be based upon economics.

Table 3 gives the economic equations used in the design of this process. The cost of the reactor, Equation (7), is dependent upon the volume; and the cost of the column, Equation (8), is a function of the number of stages. These data (Peters and Timmerhaus, 1968) are corrected to 1974 and for stage efficiency. The column diameter was essentially constant in this example and does not appear as a variable in the correlation.

Since the average flow of raw material to the process is constant, the cost of raw material R_A is fixed. The process is based on 330 days of operation annually. Revenue from the sale of product B, Equation (10), is computed at \$0.20/kg mol for material meeting or exceeding the specifications and \$0.15/kg mol for product that does not meet the specifications. It should be noted that the quantity of product is not constant, and therefore B appears in Equation (10). The annual profit is calculated as the revenue minus the sum of: (1) the cost of raw material, (2) depreciation, interest, maintenance and labor computed as 30% of the investment in the column and reactor, and (3) income taxes at 50%.

The selection of the proper volume and stages for this process is an optimization problem which can be stated as*

$$\text{MAX. } P = h(V, S, \hat{Q}, \hat{k}, \widehat{L/D}) \tag{12}$$

Subject to:

$$X_B \geqq .95$$
$$B \geqq 1.35 \text{ kg mols/min}$$
$$\hat{Q} = 0.0047 \pm 0.001 \ (\text{m}^3/\text{s})$$
$$\hat{k} = 0.0033 \pm 0.0003 \ (\text{s}^{-1})$$
$$\widehat{L/D} = 1.1 \pm .09 \times (L/D)\text{min}$$

The function h represents Equations (1) through (11). The dependability does not appear in Equation (12) since it is completely dependent upon V and S.

The variables $\hat{Q}$, $\hat{k}$, and $\widehat{L/D}$ are random variables, and therefore this is a stochastic optimization problem. Since no formal optimization technique has been established for solution of this class of problem, a direct (exhaustive) search procedure was applied. This procedure can be stated as follows:

1. Choose reactor volume V.
2. Randomly determine variable design conditions, $\hat{Q}$, $\hat{k}$, $\widehat{L/D}$.
3. Using design equations, find number of stages S to satisfy product specifications.
4. Repeat steps 2 and 3 for statistical significance.
5. Find the dependability for a given V and S as the number of times that number of stages or more was found in step 3 above, divided by the total number of trials in step 4. Since dependability is a cumulative probability, it is computed as the fraction of the total observations requiring a certain V and S. An alternative procedure (somewhat less efficient) would be to fix the volume and number of stages, simulate $\hat{Q}$, $\hat{k}$ and $\widehat{L/D}$ a number of times, and measure the dependability as the fraction of simulations which satisfy the product constraints.
6. Calculate profit for each level of dependability.
7. Repeat from step 1 until optimal design is found.

* It should be noted that V and S are not independent of $\hat{Q}$, $\hat{k}$, and $\widehat{L/D}$ and are also dependent upon one another. Therefore, complete freedom of the variables, in the usual sense, is not possible.

TABLE 1. PROCESS DESIGN EQUATIONS

$$C_{A0} = \frac{C_{AI}}{1 + \dfrac{kV}{Q}} \tag{2}$$

$$\text{or } V = \frac{Q(C_{AI} - C_{A0})}{C_{A0}\, k}$$

$$\frac{S - N}{S + 1} = .35 \left[\frac{(L/D) - (L/D)_{\min}}{L/D + 1} \right]^{-.15} \tag{3}$$

$$N \ln \alpha_{\text{avg}} = \ln \frac{(C_B/C_C)_{\text{Top}}}{(C_B/C_C)_{\text{Bottom}}} \tag{4}$$

$$(L/D)_{\min} + 1 = \sum \frac{\alpha_i C_{i\text{Feed}}}{\alpha_i - \theta} \tag{5}$$

TABLE 2. DESIGN CONDITIONS

Variable conditions

$Q = .0047 \pm .001$ (m³/s)
$k = .0033 \pm .0003$ (s^{-1})
$L/D/(L/D)_{\min} = 1.1 \pm .09$

Product specifications

$C_B \geqq .95$
$B \geqq 1.35$ (kg mols/min)

Other data

$C_{AI} = 1.0$
$\alpha_A = .4$
$\alpha_B = 1.2$
$\alpha_C = 1.0$
$MW_A = 130$
$MW_B = 60$
$MW_C = 70$

TABLE 3. ECONOMIC EQUATIONS

$$I_R = 12{,}000 + 3{,}200\ V \tag{7}$$

$$I_C = 18{,}000 + 6{,}600\ S \tag{8}$$

$$R_A = \$.06/\text{kg mol} \times 2.25 \times 475{,}000 \text{ min./yr.} \tag{9}$$

$$R_B = \$.20/\text{kg mol} \times B \times D \times 475{,}000 + \$.15/\text{kg mol} \times B \times (1 - D) \times 475{,}000 \tag{10}$$

$$P = 0.5\,[R_B - R_A - 0.3\,(I_R + I_C)] \tag{11}$$

RESULTS AND DISCUSSION

The results of the simulation for various levels of dependability are shown in Figure 2. As expected, more dependable designs require a larger column and reactor. It is noted that for each dependability contour, there is a minimum reactor volume and also a minimum number of stages. This condition occurs because of the dual product specification. In order to satisfy the product quantity restriction, there is a minimum reactor volume for each dependability. Similarly, to achieve 95% purity, a minimum number of stages is necessary. It is observed from Figure 2 that the dependability is nonlinear with respect to either volume or stages; that is, for a given number of stages a larger change in volume is required to go from 95 to 100% dependability than from 90 to 95, etc. This relationship was found to be exponential in an earlier study (Freeman and Gaddy, 1973).

It is interesting to note from Figure 2 that there is a contour for 100% dependability. Thus, the problem is one of optimization even to produce at specification all of the time.

Table 4 presents the annual profit expected for various combinations of volume, stages, and dependability. It is noted that for each level of dependability, the maximum profit occurs at the minimum number of stages and the maximum volume. For example, at 85% dependability, the profit is highest at the minimum stages of 36 and the corresponding volume of 2.7 m^3. A different volume with 36 stages would change the dependability. An increase in the number of stages would permit a smaller volume, thus tending to balance any change in investment. However, a smaller quantity of product is produced; consequently, the revenue and profit are less. With different economic parameters, the maximum profit might not always occur at the minimum stages.

A plot of the maximum profit at each level of dependability is shown in Figure 3. The optimum profit occurs at a dependability of 0.9, corresponding to 36 stages and a volume of 8.5 m^3. The curve in Figure 3 shows a decrease in profit at 85% dependability because of the discrete relationship between the dependability and number of stages. If 35.5 stages were possible at 85% dependability, a smooth curve (dashed line) might result.

The number of random samples required to achieve statistical significance (step 4 above) is of importance in a study of this type. Table 5 shows the results of various sample sizes on the relative error in dependability. This analysis is based upon the error in the mean value of the

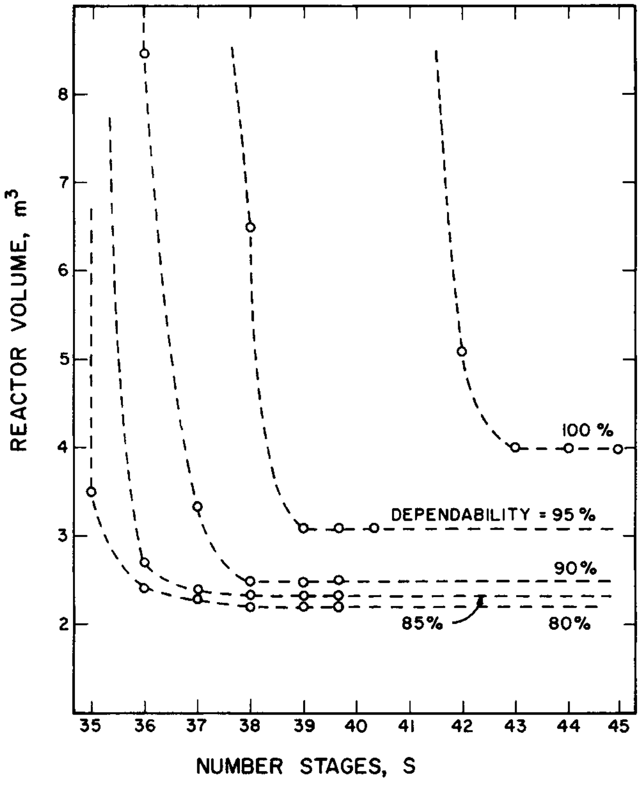

Fig. 2. Process dependability contours for various reactor volumes and tower sizes.

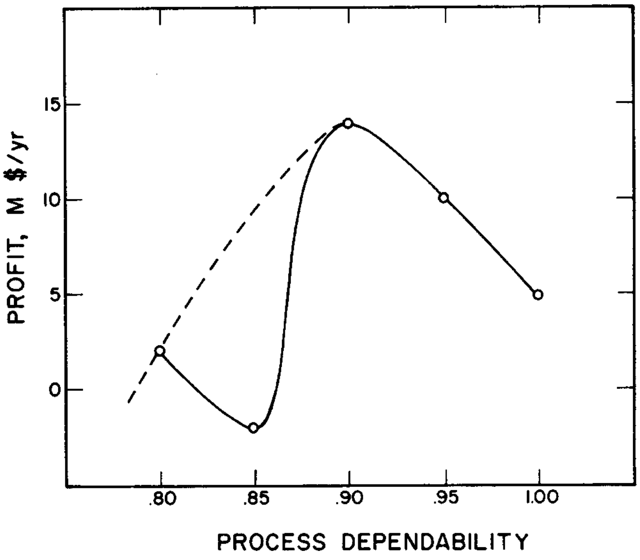

Fig. 3. Expected profit at various levels of dependability.

TABLE 4. REQUIRED DESIGN AND ANNUAL PROFIT AT VARIOUS LEVELS OF DEPENDABILITY

	Dependability Level									
	.80		.85		.90		.95		1.00	
Number stages	Reactor vol., m^3	Annual profit, m$	Reactor vol., m^3	Annual profit, m$	Reactor vol., m^3	Annual profit, m$	Reactor vol., m^3	Annual profit, m$	Reactor vol., m^3	Annual profit, m$
35	3.5	$\boxed{+2}$	—		—		—		—	
36	2.4	−6	2.7	$\boxed{-2}$	8.5	$\boxed{+14}$	—		—	
37	2.3	−8	2.3	−6	3.3	+2	—		—	
38	2.2	−9	2.3	−7	2.5	−6	6.5	$\boxed{+10}$	—	
39	2.2	−10	2.3	−8	2.5	−7	3.1	−1	—	
40	2.2	−12	2.3	−9	2.4	−8	3.1	−2	—	
41			2.3	−10	2.4	−9	3.1	−3	—	
42					2.4	−10	3.1	−4	5.1	$\boxed{+5}$
43							3.1	−5	4.0	+1
44									4.0	−1

dependability calculated from the standard deviation of grouped samples and the student distribution (Hillier and Lieberman, 1967). The error at 400 trials is seen to be 2.5% and this sample size was used in determining the dependability at each volume.

As a matter of comparison, Table 6 shows the design required at the average value of the random variables. With no safety factor applied, 33 stages and 1.9 m³ are required. This design is only 27% dependable. Adding the suggested (Peters and Timmerhaus, 1968) safety factors, the column should have 38 stages and the reactor volume should be 2.2 m³. This design is 80% dependable; however, a profit of −\$9,000 results, far from the optimum.

SUMMMARY AND CONCLUSIONS

It has been demonstrated how the concept of dependability can be used with stochastic simulation of the process variables to find the optimum overdesign of chemical processes. The example presented has three random variables and two design variables. However, the method is appropriate for higher dimensional problems.

The optimal safety factor for the reactor is 8.5/1.9 − 1 = 3.5 and for the column, 36/33 − 1 = .09. This unusual combination could hardly be arrived at by the usual methods. In some problems, dependability alone might be used to determine overdesign. However, a more general problem involves optimization using the dependability criterion. Direct search optimization procedures become tedious for these problems; and development of better optimization procedures under uncertainty should be undertaken.

NOTATION

B = product rate, kg mol/s
C_i = composition of component i, mol. frac.
C_{Af} = concentration of A in feed, mol. frac.
C_{A0} = concentration of A from reactor, mol. frac.
D = process dependability, the fraction of the time the process is required to perform at specification
$f(x)$ = probability density function of x
I_R = investment for reactor, \$
I_C = investment for column, \$
k = reaction rate constant, s^{-1}
L/D = actual reflux ratio
$(L/D)_{min}$ = minimum reflux ratio, found by Equation (5)
N = minimum number of theoretical stages, found by Equation (4)
P = annual profit, \$/yr.
Q = flow rate in reactor, m³/s
R_A = cost of raw material A, \$/yr.
R_B = revenue from sale of product B, \$/yr.
S = actual number of theoretical stages
V = reactor volume, m³
X = process variable chosen as indicative of process performance
α_i = relative volatility of component i
l = tolerance limit (specification) of process performance
θ = parameter defined by feed condition $\alpha_B < \theta < \alpha_C$

TABLE 5. ERROR ANALYSIS

No. iter.	Avg. dep. @ N = 36 V = 8.5	Std. dev. of grouped samples	Relative error in dep.
50	.92	.130	.14
100	.927	.096	.05
200	.915	.099	.04
300	.903	.089	.03
400	.907	.086	.025

TABLE 6. DESIGN BASED ON MOST LIKELY VALUES

Q = .0047 (m³/s)
k = .0033 (s^{-1})
$(L/D)/(L/D)_{min} = 1.2$
S = 33
V = 1.9 (m³)
D = .27

Adding Recommended Safety Factors (15%)

S = 38
V = 2.2 (m³)
D = .80
Profit = −\$9,000

LITERATURE CITED

Berryman, J. E., and D. M. Himmelblau, "Influence of Stochastic Inputs and Parameters on Heat Exchanger Design," *Ind. Eng. Chem. Process Design Develop.*, **12**, 165 (1973).

Chen, M. S. K., L. E. Erickson, and L. Fan, "Consideration of Sensitivity and Parameter Uncertainty in Optimal Process Design," *ibid.*, **9**, 514 (1970).

Coulter, K. E., and V. S. Morello, "Improving Onstream Time in Process Plants," *Chem. Eng. Progr.*, **68**(3), 56 (1972).

Fenske, M. R., "Fractionation of Straight-Run Pennsylvania Gasoline," *Ind. Eng. Chem.*, **24**, 482 (1932).

Freeman, R. A., and J. L. Gaddy, "Quantitative Overdesign of Pollution Control Systems," *AIChE Symp., Ser. No. 145*, **71**, 128 (1975).

Gaddy, J. L., and O. L. Culberson, "Prediction of Variable Process Performance by Stochastic Flow Sheet Simulation," *AIChE J.*, **19**, 1239 (1973).

Gilliland, E. R., "Estimation of the Number of Theoretical Plates as a Function of Reflux Ratio," *Ind. Eng. Chem.*, **32**, 1220 (1940).

Hess, S. W., and H. A. Quigley, "Analysis of Risk in Investment Using Monte Carlo Techniques," *AIChE Symp. Ser., No. 42*, **59**, 55 (1963).

Hillier, F. S. and G. J. Lieberman, *Introduction to Operations Research*, Holden-Day, San Francisco (1967).

Kittrell, J. R. and C. C. Watson, "Don't Overdesign Process Equipment," *Chem. Eng. Progr.*, **62**, 79 (April, 1966).

Lashmet, P. K. and S. Z. Szczepanski, "Efficiency Uncertainty and Distillation Column Overdesign Factors," *Ind. Eng. Chem. Process Design Develop.*, **13**, 103 (1974).

Mischke, C., "A Method of Relating Factor of Safety and Reliability," *J. Eng. Ind.*, **92**, 537 (1970).

Peters, M. S., and K. D. Timmerhaus, *Plant Design and Economics for Chemical Engineers*, McGraw-Hill, New York (1968).

Saletan, D. I., and A. V. Caselli, "Optimum Design Capacity of New Plants," *Chem. Eng. Progr.*, **59**, 69 (May, 1963).

Sprow, F. B., "Evaluation of Research Expenditures Using Triangular Distribution Functions and Monte Carlo Methods," *Ind. Eng. Chem.*, **59**, 35 (July, 1967).

Su, H., "Design by Quantitative Factor of Safety," *J. Eng. Ind.*, **82**, 387 (1960).

Svenson, N. L., "Factor of Safety Based on Probability," *Eng.*, **191**, 154 (Jan. 27, 1961).

Tayyabkhan, M. T., and T. C. Richardson, "Monte Carlo Techniques," *Chem. Eng. Progr.*, **61**, 78 (Jan., 1965).

Ufford, P. S., "Equipment Reliability Analysis for Large Plants," *Chem. Eng. Progr.*, **68**(3), 47 (1972).

Underwood, A. J. V., "Fractional Distillation of Multicomponent Mixtures," *Chem. Eng. Progr.*, **44**(8), 603 (1948).

Manuscript received October 7, 1974; revision received and accepted January 24, 1975.