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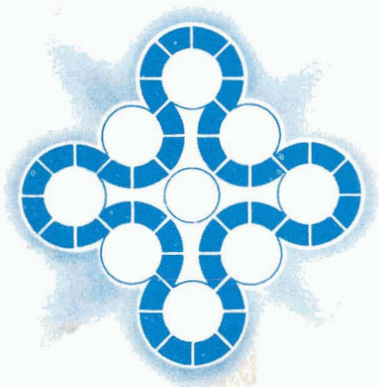
PRODUCTION OF 14 MeV NEUTRONS BY HEAVY IONS

R.M. Brugger, R.C. Young and L.G. Miller



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Mathematics and Computers
TID-4500

THE REBAL COMPUTER PROGRAM SERIES FOR LINEAR PROPAGATION OF UNCERTAINTY

BY

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ABSTRACT

The theory used for development of the REBAL computer program series for linear propagation of uncertainty in computer assisted engineering computations is given. The approximations used in REBAL are presented. Emphasis is placed on the interpretation of the input and output as calculated by REBAL. This report is written for engineers with only basic statistical background.

SUMMARY

REBAL is a computer program that establishes the statistical distribution of the output from engineering computations from the distributions of the parameters input to the engineering computations. The input distributions can represent randomly varying input or can be an expression of uncertainty in the input parameter.

REBAL is based on the theory of linear propagation of variance and thereby the output distribution is calculated rather than estimated from a sample as it is in the Monte Carlo approach. To calculate the output distribution, the partial derivatives of the output with respect to each distributed input parameter are required and are determined by REBAL by the finite difference technique.

From the output distribution, an interval estimate of the output is established. In the case of randomly varying input this interval estimate is interpreted as an interval expected to contain the actual output a specified percentage of the time. For the case for which the input is an expression of uncertainty in the input parameter, the interval estimate is expected to contain, with a specified probability, the model result that would occur if all the input parameters were precisely known. The term probability is interpreted in the latter case in a Bayesian sense.

CONTENTS

FIGURES

THE REBAL COMPUTER PROGRAM SERIES FOR LINEAR PROPAGATION OF UNCERTAINTY

I. INTRODUCTION

Modern engineering calculations involve complex sets of equations that are generally solved using digital computers. The input parameters used for the calculations are rarely accurately known. The equations used for the calculations then are transfer functions for the uncertainty associated with the input parameters, hence uncertainty is propagated through the calculations. The result is uncertainty in the output of the computation. Analysis to determine this uncertainty is important because of cost and safety contingencies. Uncertainty analysis (in conjunction with experimental data) is necessary for verification of analytical models that have input parameters that are not accurately known.

The REBAL computer program series, Routines for Error Bounds Assuming Linearity, was written to quantify the output uncertainty that results from uncertainty in the input parameters of several existing computer programs. REBAL uses these existing, unmodified computer programs as subroutines; that is, it calls them as modules. Only two portions of REBAL must be tailored to the computer program for which uncertainty propagation analysis is to be carried out; the remainder of REBAL remains unchanged. Thereby the effort necessary to extend the REBAL series to include the analysis of output uncertainty of additional computer programs is minimized.

Two types of situations can be analyzed by the techniques of linear propagation of variance that are used in REBAL. One deals with the treatment of randomly varying input and, consequently, randomly varying output; the other deals with treatment of uncertainty associated with quantities that have fixed but unknown values.

As an example of propagation of the effect of randomly varying input, a situation dealing with electrical resistors is given. Amplifiers are built using resistors taken from a lot of resistors that are known to vary in resistance. For this example the pertinent characteristics of all other amplifier components are assumed not to vary. The variation in resistance is determined by examining some, or all, of the resistors, and the probability density function (pdf) for the value of resistance of a resistor from this lot is determined. The gain of an amplifier is dependent on the resistance of the resistor used for its construction and consequently varies from one amplifier to another. Through use of the mathematical model for determining the gain of an amplifier, the pdf for the resistors, and techniques of propagation of variance, the pdf for the gain of an amplifier built using resistors from the lot can be determined. Hence, a probability statement about the gain of a given amplifier can be made. This example is one of classical propagation of variance and can be analyzed through use of REBAL.

The other type of situation that can also be analyzed by techniques of linear propagation of variance, hence REBAL, deals with the propagation of uncertainty associated with parameters that are input to engineering computations. A subjective assignment of uncertainty distributions for the input parameters is often employed. The required distributions can, however, be based entirely on experimental results or can result from a combination of experimental results

and subjective assignment. Subjective assignment of density functions is not new and is commonly used in "Bayesian Inference" techniques. The object of Bayesian methods is to use all available information whether it be sample information or information of some other origin. If data are to be used in conjunction with subjective assignment then the initial subjective distribution is called the "prior" distribution. The prior distribution is then modified to reflect the information contained in the data. The result is a posterior distribution. References 1 and 2 give a more detailed treatment.

For uncertainty propagation analysis the input parameters have fixed values; the analyst does not, however, know what these true values are. The associated uncertainty distributions are an assignment of lack of confidence, or uncertainty, the analyst has in the input parameters. Based on these input uncertainty distributions, REBAL establishes the distribution of the computational output.

In Section I general concepts are introduced and in Section II the methods used in REBAL are given. The specific equations and the approximation used in REBAL are discussed in Sections III, IV, and V. In Section VI the technique used to establish the certainty interval on the output of interest is put forth. Input and output interpretations are discussed in Sections VII and VIII, respectively. Finally, in Section IX the conclusions are presented and recommendations are made.

II. METHOD OF APPROACH

REBAL is based on the theory of linear propagation of variance[3,4,5]. Another method of analyzing output uncertainty is the Monte Carlo technique, as described in Reference 6. A main difference between the linear and Monte Carlo techniques is that in the linear approach the assumption is made that the quantitative measures of uncertainty; that is, the standard deviation and mean of the associated distribution can be calculated whereas in the Monte Carlo approach these quantitative measures are estimated from a sample.

The assumptions and limitations inherent to linear propagation of variance, and hence, REBAL are as follows:

(1) The output of the calculation as a function of each input parameter in question can be approximated validly in the vicinity of the output value that results from the mean input values, by the linear terms of a Taylor series expansion.

(2) The uncertainty in the input parameters is distributed with known mean and standard deviation.

(3) The uncertainty in the output of the computation is normally distributed.

(4) The input parameters are statistically independent.

The first assumption is illustrated in Figure 1. Here the output is shown as a function of one input variable. The term vicinity in the first assumption is defined as the range of output values resulting from input values in a domain such that this domain encloses nearly all, say 95%, of the area under the distribution. This assumption is needed so that the output as a function of each input variable can be approximated by the linear terms of a Taylor series over the range of interest. If many input variables are considered, the usual case, a hyperplane tangent to the surface generated by the range of the output is assumed to describe the output in the vicinity of the output value that results from the mean input values. In a detailed study, Ku[5] has shown the uncertainty propagation equations resulting from this assumption are accurate if (a) the percent uncertainty in the input parameter is small and (b) the second and higher order partial derivatives of the mathematical model are small when evaluated at the respective mean values of the input parameters.

The second assumption allows the input uncertainty distribution to be of any type (normal, lognormal, uniform . . .) so long as the mean and standard deviations are known. Determination of the uncertainty distributions for the input parameters is discussed in Section VII.

Assuming the output is normally distributed is necessary for interpretation of the results. The output is indeed nearly normally distributed in cases of interest as has been validated in many cases by Monte Carlo analyses and in some cases by Lapunov's Theorem[4], not to be confused with the standard central limit theorem. Cramer, as stated by Ku[5], has shown for a large number

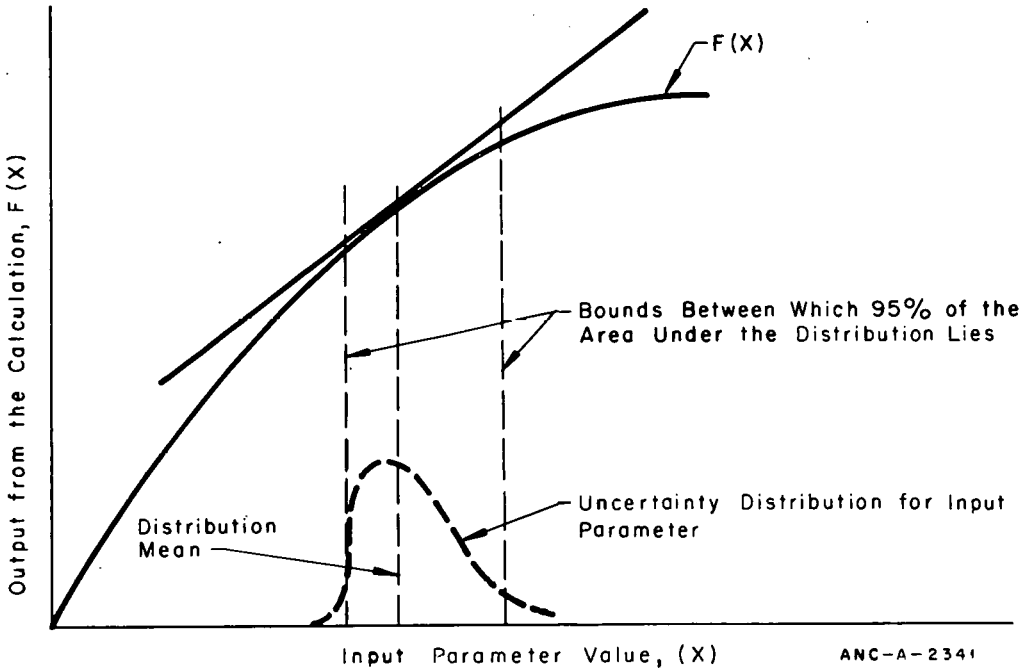


FIG. 1 ILLUSTRATION OF THE ASSUMPTION OF LINEARITY USED IN REBAL.

of input parameters that this distribution is, indeed, approximately normal. In addition, Ku[5] concludes that if conditions (a) and (b) given previously prevail and the input parameter distributions are normally distributed, the distribution of the computational output is approximately normal. This assumption of normally distributed output is precisely valid, however, only if all the input parameters are normally distributed and the output is a linear function of the input parameters.

Within the framework of these assumptions, analytical expressions can be derived for calculating the mean and the standard deviation of the output distribution (Section III). Since the output distribution is assumed normally distributed, the distribution is completely described by its mean and standard deviation. REBAL solves these expressions for the particular situation of interest and establishes the associated interval estimates, also called certainty intervals, on the output (Section VI). The input to REBAL is described in Section VII and the output in Section VIII. These descriptions are of a general nature because the specific format of the input and output depends on the particular computer-assisted calculation of interest.

III. EQUATIONS USED IN REBAL

Exact analytical determination of a certainty distribution for the output of a computer program is not feasible in cases encountered in practice. If the function for the output is expanded by the use of a Taylor series and if only the linear terms are retained, an equation for the mean and the variance of the output distribution can be obtained.

Any reasonably well behaved function of many variables can be expanded in a Taylor series about a point if the necessary derivatives exist. The full expansion is given in Reference 7. If only the linear terms are retained, the expansion of the function of interest, F, reduces to the following:

$$F(\bar{X}) = F(\bar{\mu}) + \frac{\partial F}{\partial X_1}(X_1 - \mu_1) + \frac{\partial F}{\partial X_2}(X_2 - \mu_2) + \ldots + \frac{\partial F}{\partial X_j}(X_j - \mu_j) \qquad (1)$$

where

j = the number of input parameters

$F(\bar{X}) = F(X_1, X_2, X_3, \ldots X_n)$

$X_i = i^{th}$ distributed input parameter

$(\bar{\mu}) = (\mu_1, \mu_2, \mu_3, \ldots \mu_n)$

μ_i = the mean of the distribution of the i^{th} input parameter

All of the partial derivatives are evaluated at the means of the respective input parameter distributions.

The mean of $F(\bar{X})$, $\bar{F}(\bar{X})$, is given by

$$\bar{F}(\bar{X}) = \frac{1}{K}\sum_{n=1}^{K} F_n(\bar{X})$$

where $F_n(\bar{X})$ is evaluated for one random value of the $\bar{X}$ vector. By taking the average value, the terms in Equation (1) become

$$\frac{1}{K}\sum_{n=1}^{K} F_n(\bar{X}) = \frac{1}{K}\sum_{n=1}^{K} F_n(\bar{\mu}) + \frac{1}{K}\sum_{n=1}^{K} \frac{\partial F_n}{\partial X_1}(X_{1,n} - \mu_1) +$$

$$\frac{1}{K}\sum_{n=1}^{K} \frac{\partial F_n}{\partial X_2}(X_{2,n} - \mu_2) + \ldots$$

since $F_n(\bar{\mu}) = F(\bar{\mu})$ and is a constant and $\frac{1}{K}\sum_{n=1}^{K} (X_{i,n} - \mu_i)$ approaches zero as K becomes large.

$$\bar{F}\ (\bar{X}) \approx F\ (\bar{\mu})$$

Therefore, to a first order approximation, the mean of the output distribution is given by the function evaluated at the means of each input parameter distribution.

If Equation (1) is rearranged and an average value of the sum of the squares is taken over K random observations, the following equation results.

$$\frac{\sum_{n=1}^{K} [F_n(\bar{X}) - F(\bar{\mu})]^2}{K} = \frac{1}{K} \sum_{n=1}^{K} \left[\frac{\partial F}{\partial X_1} (X_{1,n} - \mu_1) + \ldots + \frac{\partial F}{\partial X_j} (X_{j,n} - \mu_j) \right]^2 \quad (2)$$

If the limit of this equation is taken as K becomes large and each input parameter is assumed statistically independent[a] from all other input parameters, the equation becomes

$$\sigma_F^2 = \sigma_1^2 \left(\frac{\partial F}{\partial X_1} \right)^2 + \sigma_2^2 \left(\frac{\partial F}{\partial X_2} \right)^2 + \ldots + \sigma_j^2 \left(\frac{\partial F}{\partial X_j} \right)^2 \quad (3)$$

where

σ_i = the standard deviation of the i^{th} input parameter

σ_F = the standard deviation of the output variable.

---

[a] Statistical independence between input parameters implies that total or partial knowledge of any parameter does not affect the uncertainty distribution of other parameters. Specifically, statistical independence exists if the probability of Event A and Event B, $P(A \cap B)$, equals the probability of A times the probabilities of B; that is, $P(A \cap B) = P(A)\ P(B)$ (Reference 8).

IV. THE DERIVATIVE APPROXIMATION USED IN REBAL

To calculate the standard deviation from Equation (3), the partial derivatives of the output with respect to each input parameter of interest are determined. These partial derivatives are approximated as follows:

$$\frac{\partial F}{\partial X_i} \simeq \frac{\Delta F}{\Delta X_i} \simeq \frac{\bar{F} - F_i}{X_{iB} - kX_{iB}} \tag{4}$$

where

$\bar{F} \equiv$ the output value that results upon substitution of the means of all the input parameter distributions.

$X_{iB} \equiv$ The mean of the distribution of the i^{th} input parameter.

$k \equiv$ A positive factor different than unity used to perturb X_{iB} and is called the perturbation factor.

$F_i \equiv$ The output value that results upon substitution of kX_{iB} for X_{iB} into a calculation otherwise identical to the calculation of $\bar{F}$.

Since $\bar{F}$ is common to the determination of all the required partial derivatives of F, n+1 calculations of F values are required where n is the number of input parameters of interest.

In numerical analysis, difference equations in the form of Equation (4) are referred to as forward difference quotients or backward difference quotients dependent on the selection of k. Other methods, such as the centered difference quotient[9], could have been used in REBAL but all of these methods require at least 2n+1 calculations of F. Since engineering computations are generally expensive, performing n+1 calculations is more appealing than performing 2n+1 calculations.

If the result of Equation (4) is a strong function of the choice of k then the assumption of linearity given in Section II is surely violated in which case an alternative approach is to use Monte Carlo uncertainty propagation analysis. In any case, what is desired is the slope of a straight line that best approximates $F(X_i)$ over most of the range of uncertainty of X_i and not necessarily the best approximation of $\frac{\partial F}{\partial X_i}$ evaluated at the mean of the X_i uncertainty distribution (Figure 1).

V. FRACTIONAL CONTRIBUTIONS OF INPUT PARAMETERS TO THE OUTPUT STANDARD DEVIATION

The fractional contribution of each input parameter to the variance of the output is easily obtained from Equation (3). The fractional contribution to the standard deviation is, however, the quantity of interest here. As indicated by Equation (3), the terms $\sigma_i \left(\frac{\partial F}{\partial X_i}\right)$ combine to give σ_F in a manner identical to the addition of orthogonal vectors. This concept is illustrated in Figure 2 for the case of two independent input parameters. The projection, ϕ, of $\sigma_1 \frac{\partial F}{\partial X_1}$ on the σ_F vector gives the contribution to σ_F that results from uncertainty in X_1 and is equal to the vector dot product divided by σ_F

$$\phi = \frac{1}{\sigma_F}\left[\left(\sigma_1 \frac{\partial F}{\partial X_1}\,\bar{i}\right).\left(\sigma_1 \frac{\partial F}{\partial X_1}\,\bar{i} + \sigma_2 \frac{\partial F}{\partial X_2}\,\bar{j}\right)\right]$$

where $\bar{i}$ and $\bar{j}$ are unit vectors along the X and Y axes, respectively.

The fractional contribution, f_1 of X_1 to σ_F, is given by

$$f_1 = \frac{\phi}{\sigma_F}$$

Therefore

$$f = \frac{\left(\sigma_1^2 \frac{\partial F}{\partial X_1}\,\bar{i}\right).\left(\sigma_1 \frac{\partial F}{\partial X_1}\,\bar{i} + \sigma_2 \frac{\partial F}{\partial X_2}\,\bar{j}\right)}{\sigma_F^2}$$

$$= \frac{\sigma_1^2 \left(\frac{\partial F}{\partial X}\right)^2}{\sigma_F^2} \quad .$$

This argument is applicable to any number of input parameters. The general expression for the fractional contribution of the i^{th} input parameter is given by

$$f_i = \frac{\sigma_i^2 \left(\frac{\partial F}{\partial X_i}\right)^2}{\sigma_F^2} \quad .$$

Therefore, the fractional contribution of each input parameter to the standard deviation of the output is the same as the fractional contribution to the output variance.

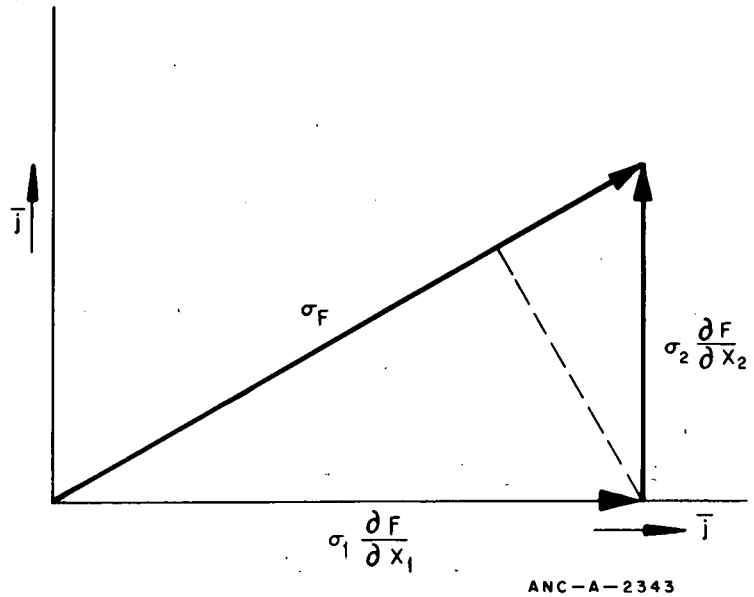


FIG. 2 VECTOR ADDITION OF COMPLETELY INDEPENDENT UNCERTAINTIES.

VI. ESTABLISHING THE CERTAINTY INTERVAL ON THE OUTPUT

The interval estimates, or certainty interval, on the output is automatically established by REBAL. A given percent, α, that is specified by the REBAL user, of the area under the output distribution is bounded and the certainty interval is thereby established. As an example, if α is set equal to 95% then the certainty interval is centered at the mean of the output distribution and extends away from the mean to points that bound 95% of the output distribution.

Since the output is assumed to be normally distributed, a factor Z_α can be defined such that $\overline{F} + Z_\alpha \sigma_F$ gives the desired certainty interval. A plot of Z_α as a function of α is given in Figure 3.

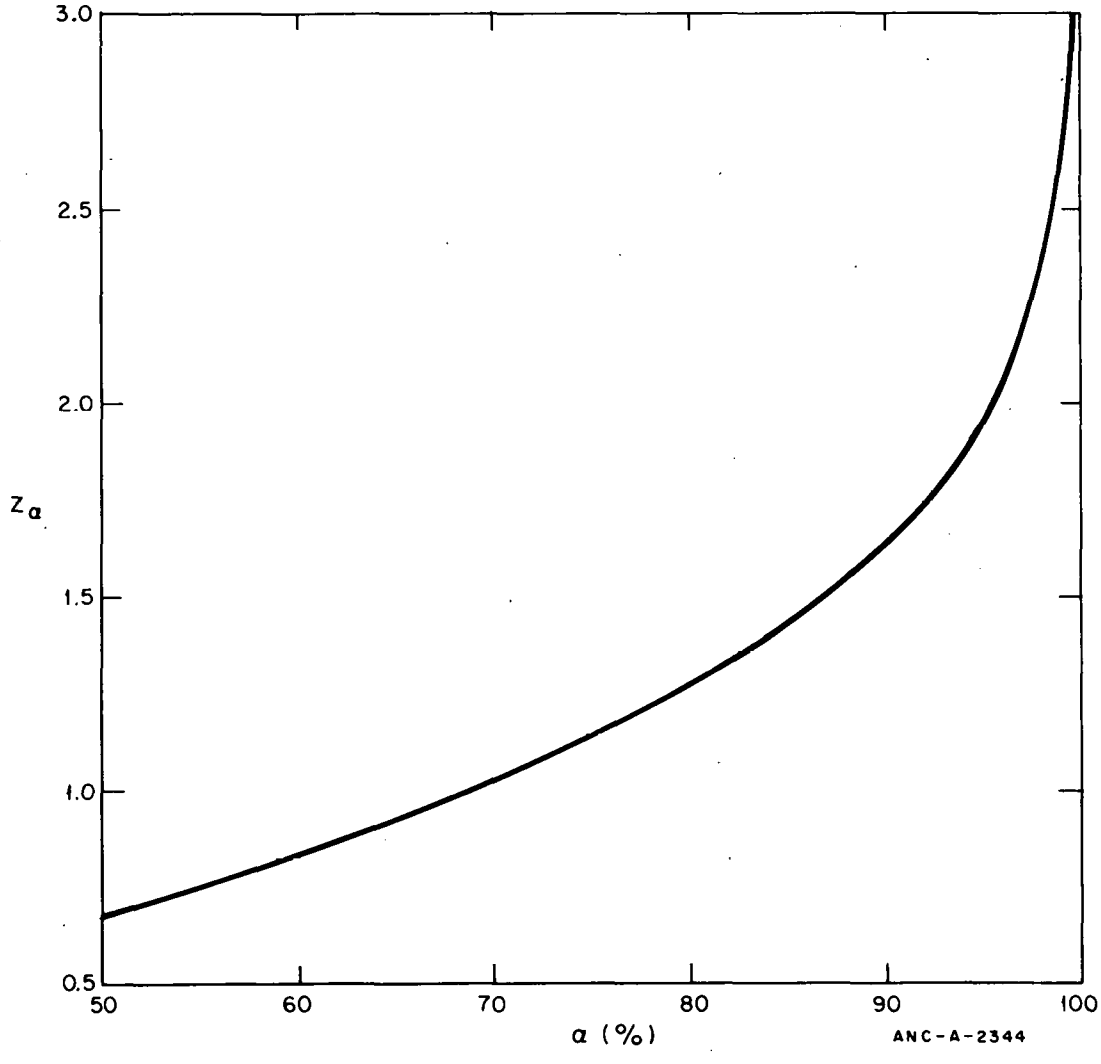


FIG. 3 THE Z_α FACTOR AS A FUNCTION OF α.

VII. REBAL INPUT AND ITS INTERPRETATION

Input to REBAL generally consists of the following:

(1) The perturbation factor for each input parameter of interest (Section IV).

(2) The standard deviation and mean of the distribution of each input parameter of interest.

(3) The value of α (Section VI).

(4) Miscellaneous input flags are required to control printout, fractional contributions, and plotting options.

The perturbation factor, k, should be chosen such that enough change is realized in the output, F, so that the partial derivative estimate is not distorted by round-off error. However, a small change is often considered to give a better estimate of the desired partial derivative. At any rate, the changed input value should be within the bounds that contain, say, 95% of the input distribution in question. Another consideration in choosing k is that kX_{iB} (Section IV) should not violate physical constraints on X_i or otherwise enter a range of X_i values that force F into a domain in which F behaves substantially different than it does in the neighborhood of F. This latter consideration in choosing k is usually automatically accounted for if kX_{iB} is within the bounds containing 95% of the distribution of X_i. Recommended values of k based on experience are [0.9 or $(1 - 2\sigma_{Xi}/X_{iB})$ whichever is larger] or [1.1 or $(1 + 2\sigma_{Xi}/X_{iB})$ whichever is smaller]. Whether k is chosen greater than 1.0 or less than 1.0 is determined by physical constraints on X_i.

The value of α used is subjectively chosen by the user. The larger α is chosen, the larger the error bands. Conventional values of α are 90% and 95%.

Determination of the standard deviations and means of the distributions of the input parameters depend on whether the inputs are random variables or are fixed but unknown quantities. These determinations are dealt with in Sections VII-1 and VII-2, respectively.

1. INPUT QUANTITIES THAT ARE RANDOM VARIABLES

If the input quantities are random variables, such as the resistance of the resistors in the example given in Section I, the input distributions are determined by standard statistical techniques. A random sample is taken from the population of each input variable and the distribution characteristics are determined. For example, if the distribution is assumed normal, then the estimate of the mean, $\bar{X}$, and the estimate of the standard deviation, s, are given by

$$\bar{X} = \frac{1}{n} \sum_{i=1}^{n} X_i$$

$$s = \sqrt{\sum_{i=1}^{n} (X_i - \bar{X})^2/(n-1)}$$

where X_i is the i^{th} value of the random sample. Further information about determining distributions from a sample is given in Reference 10.

The resulting distribution input to REBAL can be interpreted by the classical frequency interpretation. The probability, P, that a randomly chosen sample value will lie in a specified interval is equal to the area under the distribution bounded by that interval. If a large sample of N values is taken, 100 P% of the values are expected to fall within the specified interval.

2. INPUT QUANTITIES THAT HAVE FIXED BUT UNKNOWN VALUES

If the input quantities have fixed but unknown values, the uncertainty distributions input to REBAL are determined subjectively or from experimental data or both.

If experimental data alone are to be used to determine the uncertainty distribution and a large sample has been taken, that is, more than 30 samples, and the population is normally distributed, then the mean, μ, and standard deviation σ are given by

$$\mu \leftarrow \frac{1}{n} \sum_{i=1}^{n} X_i$$

$$\sigma \leftarrow \sigma^*/\sqrt{n}$$

and σ^* is estimated by s as given in Section VII-1. For smaller sample sizes the "student's t" distribution can be used[2]. Otherwise the uncertainty distributions are assigned subjectively, which is usually the case. The first steps are to:

(1) Obtain a nominal value (value estimated to be the most likely true value) for the parameter

(2) Determine the physical bounds for the parameter

(3) Subjectively obtain an appropriate distribution type (normal, uniform, . . .) for the parameter

(4) Estimate a certainty interval for the parameter (for example, the chance the true parameter value lies within a specified interval is 0.95).

To obtain a nominal value, the analyst should seek the best possible estimate of the true value of the parameter and not a "conservative" value. This best possible estimate usually serves as the mean of the input certainty distribution.

Physical bounds for the parameter can normally be determined. As an example, a reactor fuel pellet length may be constrained between 0.90 and 1.10 inches, with other fuel pellets having been discarded. (This constraint is not to be confused with engineering tolerances for the fuel pellet which in this example might be 1.00 ± 0.002 inch. Dimensions are not necessarily constrained at the engineering tolerances.)

For most uncertainty propagation analyses the input parameters are assumed to be normally distributed. The assumption of normality must be considered as simply an assumption regarding the form of a mathematical model which, at best, is an approximation to a real situation.

Many things about the normal approximation are pleasing. The distribution is symmetrical about the mean. The uncertainty in the parameter is entirely described by the standard deviation. The probability of a random value being selected is greatest for the mean value and is monotonically decreasing as a function of distance from the mean. Values further than 3σ from the mean have a very small probability of occurring (<0.3%). The distribution also has "nice" mathematical features and is well tabulated. If another distribution is used, the mean, E(X), and the standard deviation, σ, must be determined by standard techniques. These determinations can become tedious but they are always given by

$$\sigma = \sqrt{E(X^2) - [E(X)]^2}$$

where

$$E(y^n) = \int_{-\infty}^{+\infty} y^n g(y)\,dy$$

$g(y) \equiv$ the probability density function of y.

If the uncertainty distribution is assumed to be normally distributed then the mean is generally assumed to be the nominal parameter value. An approximation of σ can be obtained in almost any situation. The first technique to be discussed requires values a and b to be estimated -- the value, a, being a lowest parameter value and b being a highest parameter value such that a 99.7% chance exists that the actual parameter lies between a and b. Then

$$\sigma \leftarrow \frac{\text{Max}[(\mu-a),\ (b-\mu)]}{3} .$$

If a and b are chosen such that a 95% chance exists that the actual parameter is included in the interval, a to b, then

$$\sigma \leftarrow \frac{\text{Max}[(\mu-a),\ (b-\mu)]}{2}$$

where Max [X,Y] denotes that the maximum value of X or Y is chosen. The maximum value is necessary because, whereas the normal distribution is symmetrical, the analyst may not select values a and b that are equidistant from the mean. By choosing the maximum distance from the mean, a degree of conservatism is factored into most cases because ultimately the uncertainty bounds on the output parameter will be somewhat larger.

Another approach that is conceptually equivalent to the estimation technique presented is to estimate the percent uncertainty in the parameter from experience. In this case $\sigma = \frac{B\mu}{Z_\alpha}$ where 100 B% is the maximum percent uncertainty in the parameter expected with confidence α. Z_α is the factor in Figure 3 corresponding to α.

A similar estimate for σ can be obtained for other distributions. Expressions for these estimates are given for several simple distributions in Figure 4.

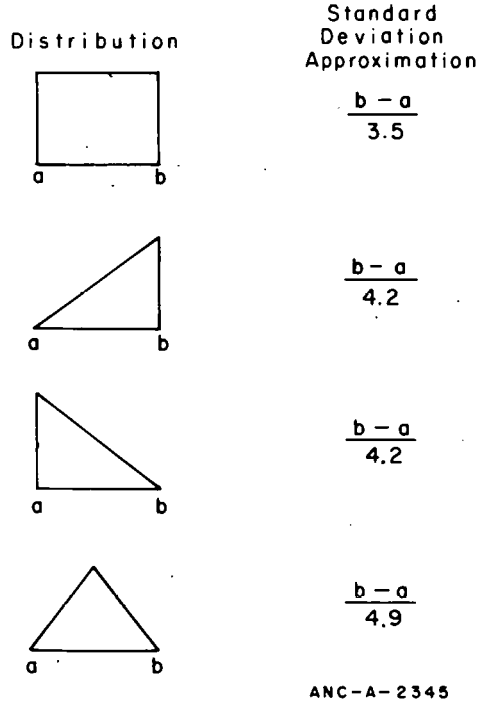


FIG. 4 ESTIMATES OF STANDARD DEVIATIONS FOR VARIOUS TYPES OF DISTRIBUTIONS.

The analyst responsible for establishing certainty intervals can solicit uncertainty distributions from those persons qualified to subjectively assign these distributions. To aid in obtaining the distribution, forms can be used such as the one given in Figure 5. To use the form shown in Figure 5 the analyst first fills in the parameter description (1) and often the best point estimate, μ, (not conservative) of the parameter (3). The qualified individuals then select an appropriate distribution type (2) with uncertainty bounds, a (4) and b (5) with an estimate of the chance P that the true parameter lies between a and b (6). Details of establishing these "prior" distributions are given in Reference 1.

Often an input parameter will be input to the computation as a correlation, W(X), that is a function of an output parameter X. As a case in point, the thermal conductivity of a material can be considered as a function of temperature in a calculation to determine the temperature. Such correlations are replaced by $\rho W(X)$, where ρ is a constant that "corrects" the correlation to give the true value. The correct value of ρ is not known. An uncertainty distribution is assigned to ρ and the uncertainty in W(X) is thereby transferred to ρ.

ESTIMATE OF PARAMETER UNCERTAINTY BASED ON ENGINEERING JUDGEMENT

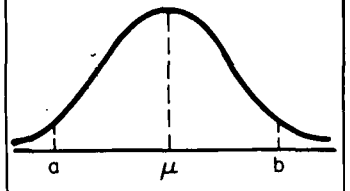
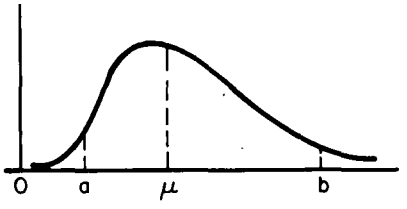
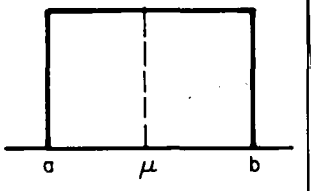
(1) Parameter Description: _____

_____

_____

_____

DISTRIBUTIONS CHARACTERISTICS
(select appropriate type)

		Normal	Log-Normal (asymmetric)	Uniform	Other
(2)	Type				
(3)	μ				
(4)	a				
(5)	b				
(6)	P				

(7) Comments: _____

_____

μ ≡ Best point estimate (not conservative)

a ≡ Lower uncertainty bound

b ≡ Upper uncertainty bound

P ≡ Estimated chance that the true parameter value is between a and b

(8) Analyst: _____ Date: _____

FIG. 5 SAMPLE FORM FOR ESTIMATING PARAMETER UNCERTAINTY.

ANC-A-2346

VIII. REBAL OUTPUT AND ITS INTERPRETATION

The output from REBAL can consist of the following:

(1) The most probable output value with certainty intervals specified

(2) The partial derivative of the output with respect to each input parameter

(3) The fractional contribution of each input parameter to the output certainty interval.

If the normal computational output is a function of one or more variables, then all of the REBAL output is obtained as a function of these same variables. For example, if the normal computational output is temperature and the temperature is obtained as at various mesh points and time steps, then the certainty intervals, partial derivatives, and fractional contributions can be obtained at these mesh points and time steps.

1. OUTPUT QUANTITIES THAT ARE RANDOM VARIABLES

If the parameter distributions input to REBAL are for random variables (Section VII-1), then the output distribution is a probability density function for a random variable; hence, a classical probability statement can be made. For example, if $\alpha = 0.95$, then the probability that the actual value lies between $\overline{X} \pm 1.96\sigma$ is 0.95.

2. OUTPUT QUANTITIES THAT HAVE FIXED BUT UNKNOWN VALUES

If the parameter distributions input for REBAL are an expression of uncertainty about the true value of the parameter, then the output distribution is the distribution of the true result of the computation. The true result of the computation is defined as the computational output that results if the exact true value of each parameter input to the computation were used. The true result of the computation, Y', is a fixed but unknown quantity. The interval estimate of, Y, the model output, is an interval that is expected to contain Y'. The output distribution and, consequently, the interval estimate of Y then cannot be interpreted in a frequency, or classical, sense because regardless of the interval chosen, the true result of the computation either lies in the interval all the time or it never does. Consequently, a classical, or frequency, probability statement cannot be made about a certainty interval, but rather the interval is interpreted in a Bayesian sense as described by Hays and Winkler [1]. The distribution of Y is defined as a certainty distribution and is interpreted analogously to the

uncertainty distributions for input parameters. If an interval, a to b, is established that bounds a percent of the output distribution, then an α percent chance exists that the true result of the computation lies in the interval a to b. The interval a to b is called the certainty interval. For example, if $\sigma = 95\%$, the probability that Y' lies in the interval $\bar{Y} \pm 1.96\sigma$ is 0.95. The word "probability" is interpreted here in a Bayesian sense [1].

IX. CONCLUSIONS

REBAL is a computer program capable of establishing uncertainty bounds on the output of computer assisted engineering computations. These uncertainty bounds that result from uncertainty in the input parameters can be determined for a wide variety of types of computations. REBAL requires that the computer program normally used for the computations be available. Although REBAL is intended for immediate application to uncertainty propagation analysis, it is also applicable to analysis of the effects of randomly varying parameters on predicted output.

The main limitations to REBAL are having to:

(1) Express the computational output as a linear function of each input parameter over the range of uncertainty associated with the respective input parameters

(2) Subjectively assign the uncertainty distribution to the input parameter of interest in some cases

(3) Assume the uncertainty distribution of output of the computations is normally distributed

(4) Assume the input parameters are statistically independent.

To improve the theoretical basis of REBAL, development of the following is recommended:

(1) Techniques to mitigate the preceding limitations with regard to linearity, independence, and distributions

(2) Methods to reduce the cost of determining the necessary partial derivatives.

The output from REBAL is useful not only as an expression of confidence that an interval estimate of the output contains the true value, but also as input to statistical tests used for verification of the computational model based on experimental results as well. Establishing a certainty distribution on the computational output allows the computational analytical model to be free from the responsibility, during the model verification tests, for output errors that result from error in the input parameters.

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