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RESPONSE SURFACE TECHNIQUES DEVELOPED FOR PROBABILISTIC ANALYSIS OF ACCIDENT CONSEQUENCES

J. K. Vaurio

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J. K. Vaurio
Argonne National Laboratory
Argonne, Illinois 60439
(312) 972-4689

ABSTRACT

Response surface techniques have been developed for obtaining probability distributions of the consequences of postulated nuclear reactor accidents. In these techniques probability distributions are assigned to the system and model parameters of the accident analysis. A limited number of parameter values (called knot-points) are selected and input to a deterministic accident analysis code. The results of the deterministic analyses are used to generate analytical functions (called response surfaces) that approximate the accident consequences in terms of selected system and model parameters. These analytical functions are then used in a Monte-Carlo type simulation to calculate probability distributions and related characteristics of the consequences. The use of response surfaces leads to considerable savings in computer time in comparison to direct simulation.

The probabilistic response surface methodology reported in this paper includes new knot-point selection schemes and response surface functions, functional transformations of both parameters and consequence variables, smooth synthesis of regionwise response surfaces and the treatment of random conditions for conditional distributions. The computer code PROSA developed for implementing these techniques is independent of the deterministic accident analysis codes. It can also be used for direct simulation of general analytical functions. The significance, accuracy and other merits of these features are discussed and typical results are presented for illustration purposes.

I. INTRODUCTION

The development of response surface techniques for nuclear reactor safety analysis is a relatively new aspect in the probabilistic safety methodology[1-5]. In general terms, the problem is to find the probability distribution of an accident consequence variable that is a function of many other random variables, system and model parameters. The functional relationship between a consequence variable and the input parameters is not known in analytical form but only through numerical mechanistic (deterministic) accident analysis codes. For the purpose of alleviating the obstacle of long-running computer programs in connection with a Monte-Carlo type simulation, probabilistic response surface

techniques and a related computer code PROSA have been developed at ANL. In this procedure, probability distributions are assigned to the input parameters, and combinations of parameter values are chosen from these distributions. These combinations of parameter values are then input to a deterministic accident analysis code. The results of these deterministic consequence analyses are used to generate response surfaces for the consequences as functions of the selected system and model input parameters. These approximating functions are then used to generate the probability distributions and joint distributions of the consequences, with random sampling being used to obtain values for the accident parameters from their distributions. This use of response surfaces leads to considerable savings in computer time in comparison to direct simulation.

The PROSA code is designed to be independent of any particular accident analysis codes. It can be linked with practically any code that provides "data points" for the response surface technique. An early version of the PROSA code has been previously applied to problems on fast reactor core disruptive accidents[4] and sodium fires,[6] demonstrating that it can be linked with different types of accident analysis codes. This paper can be viewed as a continuation to Ref. 7 in which many features of the PROSA code were described in detail. In Section II the basic response surface techniques of Ref. 7 are summarized. Section III describes the new knot-point selection schemes and response surface functions, functional transformations of parameters and consequence variables, weighting of regionwise response surfaces and the treatment of random conditions for conditional distributions. The significance, accuracy and other merits of the above features are discussed and typical results are presented for illustration purposes. A summary and future development needs are presented in Section IV.

II. BASIC RESPONSE SURFACE TECHNIQUES

The consequences of interest, ζ, which might include, for example, accident energetics and degrees of core and vessel damage, depend on many system and model parameters, $z_1, z_2, \ldots, z_n$,

$$\zeta = \zeta(z_1, z_2, \ldots, z_n) \equiv \zeta(\bar{z}) \quad . \tag{1}$$

The statistical variations of the parameters, z_i, which include reactivity coefficients, heat transfer parameters etc., cause variations in ζ. It is possible, in principle, to sample values of the parameters, z_i, from their probability distributions and to calculate ζ for a sufficient number of cases using comprehensive accident analysis codes. However, the long computing times of such codes often prevent this direct simulation. With response surface techniques the idea is to find a multivariate analytical approximation, $\tilde{\zeta}$ to ζ, and perform the accident simulations for randomly selected values of $\bar{z}$ with $\tilde{\zeta}$. Systematical techniques for minimizing the error $|\zeta - \tilde{\zeta}|$ in the important domain of $\bar{z}$ space are presented in section III.

Starting from a second-degree response surface, the approximation of a given consequence, $\zeta(\bar{z})$, as a function of the accident parameters, $z_1, \ldots, z_n$, has the following functional form:

$$\tilde{\zeta}(\bar{z}) = A + \sum_{j=1}^{n} \left\{ \left[B_j + C_j(z_j - z_{j0}) + \sum_{k=j+1}^{n} D_{jk}(z_k - z_{k0}) \right] (z_j - z_{j0}) \right\} \quad . \tag{2}$$

To determine the unknown coefficients, a set of $1 + 2n + [n(n-1)/2]$ knot-points, $\bar{z}$, is selected at which the approximation, $\tilde{\zeta}(\bar{z})$, is made equal to the actual values of $\zeta(\bar{z})$ calculated by a deterministic accident analysis code.

The coefficients of Eq. (2) are

$$A = \zeta_0 \quad ,$$

$$B_j = R_{j1} \cdot (z_{j0} - z_{j2}) + R_{j2} \cdot (z_{j0} - z_{j1}) \quad ,$$

and

$$C_j = R_{j1} + R_{j2} \quad ,$$

where

$$R_{j1} = \frac{\zeta_1(j) - \zeta_0}{(z_{j1} - z_{j0})(z_{j1} - z_{j2})} \quad ,$$

$$R_{j2} = \frac{\zeta_2(j) - \zeta_0}{(z_{j2} - z_{j0})(z_{j2} - z_{j1})} \quad ,$$

and

$$D_{jk} = \frac{\zeta_0 + \zeta_{11}(j,k) - \zeta_1(j) - \zeta_1(k)}{(z_{j1} - z_{j0})(z_{k1} - z_{k0})} \quad , \tag{3}$$

where $\bar{z} = \bar{z}_0 = (z_{10}, z_{20}, \ldots, z_{n0})$ is the reference point, z_{j1} and z_{j2} are two other selected values of z_j for all $j = 1, \ldots, n$, and

$$\zeta_0 = \zeta(\bar{z}_0), \; \zeta_1(j) = \zeta(z_j = z_{j1}),$$

$$\zeta_2(j) = \zeta(z_j = z_{j2}), \; \zeta_{11}(j,k) = \zeta(z_j = z_{j1}, z_k = z_{k1}) \quad .$$

The components of $\bar{z}$ not explicitly given as arguments of $\zeta(\cdot)$ have their reference values, $z_\ell = z_{\ell 0}$.

The knot-point coordinates z_{j0}, z_{j1} and z_{j2} are selected so that z_{j0} is taken as the mean value of z_j, and a user-specified probability truncation limit, P*, is used to calculate z_{j1} and z_{j2} from the conditions,

$$\int_{z_{j1}}^{\infty} f_j(z_j)dz_j = \int_{-\infty}^{z_{j2}} f_j(z_j)dz_j = P^* \quad , \tag{4}$$

where $f_j(z_j)$ is the probability density function of z_j. The value of P* depends on the problem at hand. If a certain safety characteristic has to be studied within the 99 per cent confidence level, a natural choice is P* = 0.01. Eight different distributions are available in PROSA, including uniform, normal, truncated normal, exponential, beta and log-normal distributions.

The knot-points of Eqs. (3) and (4) are illustrated in Fig. 1.A. In this case a single polynomial is used to represent a consequence in the entire parameter space. In the following this is called a single-quadrant response surface (SQ).

The second scheme, illustrated in Fig. 1.B, provides additional knot-points so that separate response surfaces can be generated for each quadrant of Fig. 1, for all pairs z_j, z_k. Equation (3) can be used in each quadrant separately. This combination of regionwise response surfaces is called a multi-quadrant surface (MQ). MQ is expected to more accurately predict the true consequence values than SQ. However, the number of deterministic calculations required to generate the response surfaces is larger, given by $1 + 4n + 2n(n - 1)$.

In the simulation phase, the coefficients to be used for a particular combination of input parameters (sampled from their distributions) are uniquely determined by the quadrants into which these parameters fall.

Sensitivity/importance measures[7] are used to organize the individual parameters and the cross terms, respectively, in their orders of importance. These indicators can be used to eliminate less important input parameters to focus the more detailed scheme of Fig. 1.B on the important parameters.

The calculation of the mean values, standard deviations and higher moments of both parameters and response surfaces, the treatment of correlated input parameters and the calculations of conditional distributions are described in Ref. 7. The distributions are obtained in the forms of histograms with 12 and 26 categories. No time-consuming sorting is used in calculating the histograms: every sample is subtracted by a reference value

and divided by the category width to obtain the category address. Currently, the PROSA code can analyze up to six consequence variables as functions of up to 12 input parameters, simultaneously. When computer times are quoted in the following, the computer used is an IBM 370/195. A typical running time is 1000 simulations per second with six consequences, and six parameters.

III. ADVANCED TECHNIQUES

1. Knot-point Selection

Two basic knot-point selection schemes were described in section II. They are illustrated in Fig. 1.A and B and are called single- and multiquadrant knot-point selection schemes, respectively. The following options are also available:

a. Knot-points with randomly-selected coordinates can be used. The scheme is illustrated in Fig. 1.C but it is not limited to two dimensions.

b. The knot-point selection distributions may be completely different (in all cases of Fig. 1) from the true probability distributions of the parameters. The latter are needed, of course, in the Monte Carlo simulation part of the analysis.

The first feature allows third-degree response surfaces to be fitted to the data whereas the schemes A and B only allow up to second-degree polynomials.

The second feature allows the knot-points to be selected from the region where the response surface has to be most accurate. Thus, importance distributions (that can be found as conditional distributions of the input parameters[7]) can be used for selecting the knot-points. The second feature also means that no separate weighting is necessary in the least-squares fitting of a response surface, since selecting the knot-points by a distribution actually performs the weighting. Further, sensitivity studies with different sampling distributions can be made without additional deterministic analyses.

2. Response Surfaces

The single- and multiquadrant response surfaces, referred to as SQ and MQ, respectively, are obtained by the interpolation equations (3). Least-squares fitting with associated error-analysis techniques provide following features:

a. A multivariate second-degree response surface can be fitted to the systematical knot-points of Fig. 1.B. This surface is denoted by MQF.

b. Multivariate second- and third-degree response surfaces can be fitted to the random knot-points of Fig. 1.C. These surfaces are denoted as RF2 and RF3, respectively.

c. Maximum positive and negative errors as well as the mean-square error of the fitted response surfaces are calculated in the knot-points. This provides a convenient means to estimate the accuracy and adequacy of response surfaces.

Not only the accuracy, but also the number of knot-points needed (= number of deterministic accident analyses) is an important factor directly related to the cost of the analysis. Table I lists the minimum number of knot-points for the response surfaces SQ, MQ, MQF, RF2, and RF3 as functions of the number N of input parameters. The number $FC = 2^N + 2N + 1$ is given for comparison, since it would be the number of knot-points in a factorial composite design.[8]

Table I. Minimum Number of Knot-Points for the Response Surfaces[a]

	Number of Knot Points			
N	SQ and RF2	MQ and MQF	RF3	FC
1	3	5	4	(3)
2	6	13	10	9
3	10	25	20	15
4	15	41	35	25
6	28	85	84	77
10	66	221	286	1045
15	136	481	816	32799

[a]The acronyms N, SQ, RF2, etc., are defined in the text.

The simplest response surfaces, SQ or RF2, are normally used when N is large. The more refined surfaces are used with small N, after the less important parameters have been eliminated. Concerning the accuracy, we expect RF2 to be more accurate than SQ in the central part of the distribution, but SQ may be more accurate in the tail area. This follows from the knot-point selection schemes. As a second-degree surface, MQF cannot be much better than RF2 or SQ but it provides conservative upper limits for the errors of MQ. MQ and RF3 should be superior to the others, since they are most flexible in predicting the true functionality of the consequence variables.

To verify the above expectations, the steady state maximum fuel temperature and the maximum clad temperature in a reactor with cylindrical fuel elements was selected for an example. The equations for these quantities are well known[9] and complicated enough not to reveal any linear or quadratic dependence in advance. This example has been used before in another context,[10] and the input parameters and their distributions are taken from Ref. 10.

The mean values and higher central moments were first calculated with different response surfaces. The mean values and the variances are relatively accurate for all response surfaces, but the third and fourth moments are most accurate with MQ and RF3. The higher the moment, the more erroneous the values generated by RF2 and SQ. These results reflect the fact that the first two moments usually depend on the central part of the distribution, where all response surfaces are relatively accurate, whereas higher moments depend on the tails, where MQ and RF3 more accurately predict the true function.

When the accuracy of the fitted surfaces was analyzed in their own knot-points, the errors of RF3 were smaller by an order of magnitude than the errors of RF2 and MQF. However, the errors of both RF2 and RF3 were large in the systematical knot-points of Fig. 1.B, even larger than the errors of MQF. The errors of MQ are zero, of course, in the knot-points of Fig. 1.B.

The lower tails of the fuel-temperature distribution are presented in Fig. 2, obtained with different response surfaces. The remarkable accuracy of the MQ surface may be associated to the following features:

a. MQ is in fact a combination of many regionwise response surfaces and therefore flexible to fit to the data.

b. The knot-points for MQ emphasize the tail areas of the distributions.

c. One or two parameters often explain most of the variation; three-parameter interaction terms are seldom important.

The random knot-points for RF2 and RF3 could also be selected from a wider distribution, thereby making these surfaces more accurate in the tail areas.

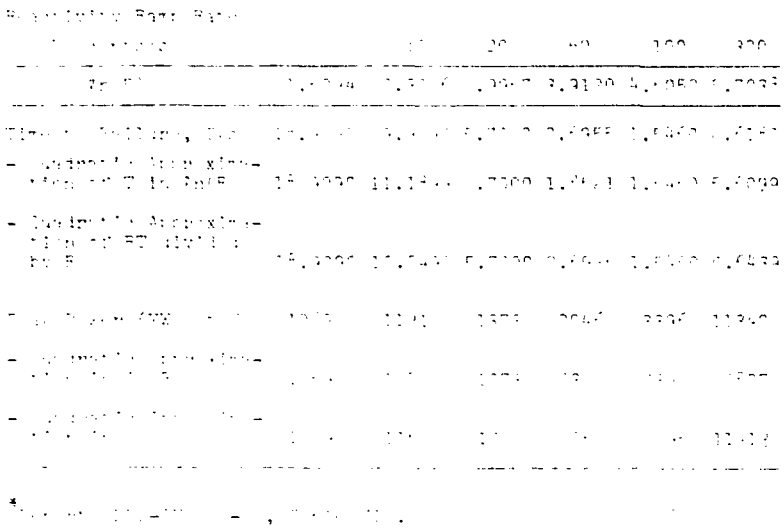
What can be said about the theoretical accuracy of MQ compared to that of the fitted surface MQF? The latter can be estimated from the residual errors of the least-squares fit. It seems that the theory is readily available only for a one-dimensional (one parameter) case and requires an estimate for the third derivative of ζ in the interpolation interval.[11] It can be shown, for example, that if ζ is a third-degree polynomial around the reference point and ε is the third-degree term, then the maximum error of MQF is $0.25\ ||\varepsilon||$ and that of MQ is $0.05\ ||\varepsilon||$, where $||\varepsilon||$ is the maximum absolute value of ε in the interval. (Equally spaced knot-points are assumed in this case.)

3. Functional Transformations

The accuracy of a response surface depends on the higher order derivatives of the consequence variable.[11] To improve the accuracy, the consequence function can be smoothed by functional

transformations. The purpose of making transformations is to be able to use a response surface of simple form in the transformed variables rather than a more complicated one in the original variables.[12] Table II illustrates the efficiency of logarithmic and product transformations in estimating the time of pin failure, T, and the peak power in case of a reactivity transient in the Fast Flux Test Facility. The ramp rates of 5, 20 and 100 cents/s were selected as knot-points for this one parameter case. The accuracy of different approximations at the ramp rates 10, 50 and 300 cents/s can be compared in Table II. Note, for example, that ℓn(T) is an almost linear function of ℓn(R).

Table II. Quadratic Approximation of the HEDL-TOP Study*



*

This example illustrates that a flexible set of functional transformations is a necessity for efficient response surface techniques. The following transformations are available in the PROSA-code:

$$
\begin{aligned}
&\text{a.} \quad y = (x - a)^b && , \quad b \neq 0 \quad ; \\
&\text{b.} \quad y = \ell n(x - a) && , \quad x > a \quad ; \\
&\text{c.} \quad y = \exp\left(\frac{x - a}{b}\right) && , \quad b \neq 0 \quad ; \\
&\text{d.} \quad y = \arctan\left(\frac{x - a}{b}\right) && , \quad b \neq 0 \quad ; \\
&\text{e.} \quad y = \frac{x - a}{x - b} && , \quad a \neq b \quad ;
\end{aligned}
\tag{5}
$$

where x is the original parameter or consequence and y is the transformed parameter or consequence, respectively.

The constants a and b of the transformations should be selected such that the residual errors of the consequences are minimized or reduced to a satisfactory level. It should be noticed that only the surface fitting part of PROSA is needed when searching for optimal transformations: no additional accident simulations or Monte-Carlo calculations are needed. The residual errors of each trial appear on the output. Due to the low cost of running PROSA, this searching process is economically feasible.

Transformations have been applied to the fuel temperature problem used in Fig. 2. The maximum positive and negative errors of the fitted response surface MQF of the maximum fuel temperature without any transformations are +29.2°C and -65.1°C. With the logarithmic transformation b. for the fuel temperature, the errors are +11.0°C and -39.8°C. With an exponential transformation c. for the fuel thermal conductivity, the errors are +11.1°C and -36.2°C, respectively. When both transformations are combined, the errors are only +3.4°C and -18.2°C, respectively. These errors are small compared to the standard deviation 160°C of the maximum fuel temperature. (The mean value is 1290°C in this example.)

4. Weighting Regionwise Response Surfaces

The regionwise response surfaces MQ, associated with Fig. 1.B, are multivariate second-degree polynomials with coefficients different in different regions ("quadrants") of the parameter space. The response surface is continuous at the region boundaries, but the derivatives may be discontinuous. To make the derivatives also continuous and to improve accuracy, a weighting method has been developed that makes the resultant surface a smooth synthesis of the regionwise surfaces. The same purpose could be achieved by using so-called spline functions for functions of one variable, but the theory of splines is not yet well-developed for functions of many variables.

With weighting, the coefficients of the quadratic response surface are continuous functions of the parameters. For example, the linear-term coefficients B_j of the resultant surface are

$$B_j = \left[W_{j4}(z_j)B_{j4} + W_{j0}(z_j)B_{j0} + W_{j3}(z_j)B_{j3}\right]/(W_{j4} + W_{j0} + W_{j3}) \quad , \qquad (6)$$

where B_{j4} is obtained from data in the knot-points z_{j2}, z_{j4}, z_{j0} of Fig. 1.B, B_{j0} in the knot-points z_{j4}, z_{j0}, z_{j3} and B_{j3} in the knot-points z_{j0}, z_{j3}, z_{j1} and

$$W_{jr} = \exp\left[-(z_j - z_{jr})^2/(2R_j^2)\right] \quad , r = 0,3,4,$$

$$R_j = \rho(z_{j1} - z_{j2})/2 \quad . \qquad (7)$$

A similar weighting principle is performed for the C_j-and D_{jk}-coefficients.

Studies with third-degree surfaces have indicated that optimal value for ρ is about 0.33. With $\rho = 0.33$, the maximum error of the synthesis response surface is one-third of the maximum error of the individual regionwise surfaces (which in turn are by a factor of 5 more accurate than MQF, as indicated in section III.2). In general, the optimal value of ρ depends on the form of the actual surface. Numerical studies indicate that values between 0.3 and 0.4 generally improve the accuracy. Smaller values do not perform efficient smoothing and larger values destroy the flexibility by averaging too much. Use of the weighting routine increases the computer running time by about 30 per cent.

Transformations reported in the previous section may be used with any response surface. With MQF, after a good transformation has been found, final refinement of the response surface can be made by weighting MQ. Fig. 3 illustrates the effect of weighting on the distribution of the reactor power in a loss-of-flow accident studied in Ref. 7. The weighted response surface is denoted by MQW. An effective transformation would bring all the distributions of Fig. 3 close to each other.

5. Function Sampling

If the interesting variables ("consequences," from our point of view) are known in analytical form, they can be programmed directly into a subroutine of PROSA. In this case, no external deterministic calculations are needed. The values are calculated in every simulation cycle directly from the equations without any response surfaces. The distributions so obtained are exact, in principle, the accuracy being determined by the sample size only. This feature is useful in safety areas such as reliability analysis where interesting quantities are known in analytical form.

This technique was applied to obtain the exact distribution in Fig. 2. As another example, the unavailability of the sample fault tree of Ref. 13 was analyzed, essentially dublicating the results. Different failure classes (single component failures, double component failures, test and maintenance contribution, common mode failures and system failures) can be analyzed simultaneously. The computer running time in this case was 10s for 10000 simulations (IBM 370/195). Compared to the SAMPLE program used in Ref. 13, PROSA has a different selection of input distributions, can handle partially correlated input parameters and forms the histograms without comparative sorting.

6. Random Criteria for Conditional Distributions

In certain cases interesting consequences (e.g. failures) appear only when some criteria function exceeds a critical value. A procedure for calculating conditional distributions under such criteria is available and has been extended for more general problems in which the criteria values (conditions) are random variables. The importance of this feature can be illustrated by an example from structural mechanics. Even if a structure, e.g., a primary vessel, is designed for a specific load, the actual strength of the structure is a random variable. When evaluating failure probabilities, and distributions of other consequences such as the amount of leakage when failure occurs, we must treat not only the loads but also the failure criteria as random variables. The PROSA code does this automatically in every simulation cycle without a separate evaluation of the overlapping of the stress and strength distributions. Studies of this kind are important for evaluating the margin of safety or the degree of conservatism in structural-design guides. Current analytical stress-strength interference techniques[14] only address the question of failure probability, not the concurrent distributions of third variables such as the leakage.

IV. SUMMARY

In summary, response surface techniques have been developed with several optional knot-point selection schemes, interpolation schemes and fitted second- and third-degree surfaces. Techniques have also been developed for estimating and improving the accuracy of the surfaces by transformations and by smoothing. The relative merits of these features have been discussed, including the options for function sampling and for conditional distributions with random criteria. Typical results have been presented for illustration purposes. Quantitative error estimation capability makes these techniques a sound basis for probabilistic analysis of the consequences of postulated accidents in cases where direct simulation is too expensive.

Further development is needed in the area of threshold effects when the consequence variable or its derivative is discontinuous and different response surfaces are needed on different sides of the threshold. Another area for future development is the identification of most important parameters of large accident analysis codes. Table I indicates that response surface techniques are feasible if the number of variable input parameters is relatively small. Variants of so called "group screening" techniques should be useful for identifying important parameters from relatively few randomly selected data points.

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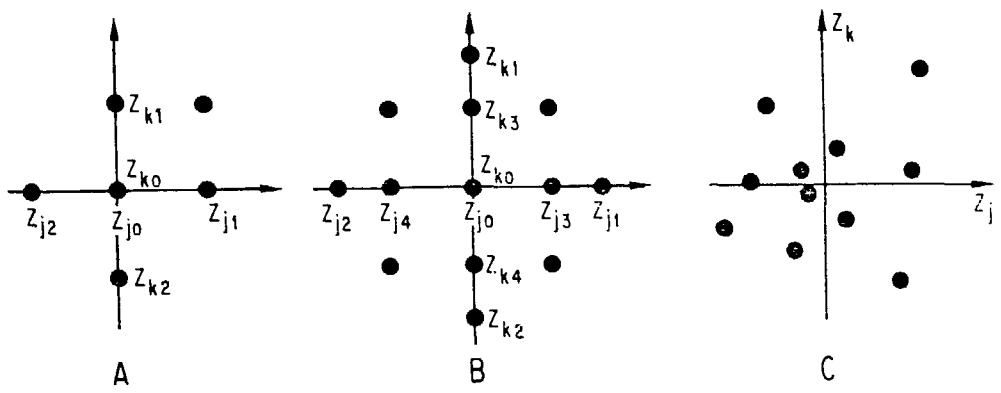

Fig. 1. Knot-point Selection Schemes

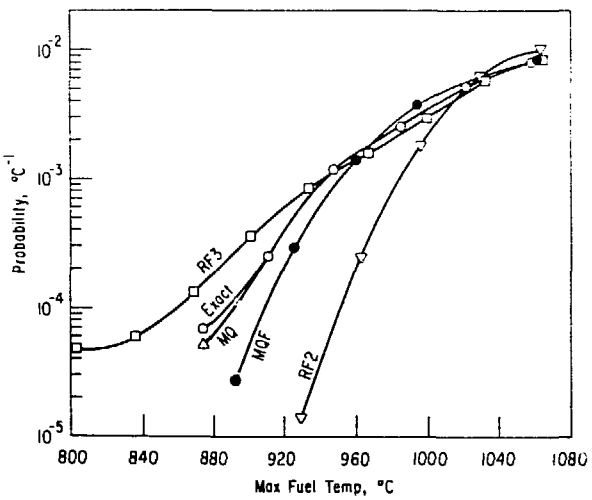

Fig. 2. Probability Densities Obtained with Different Response Surfaces

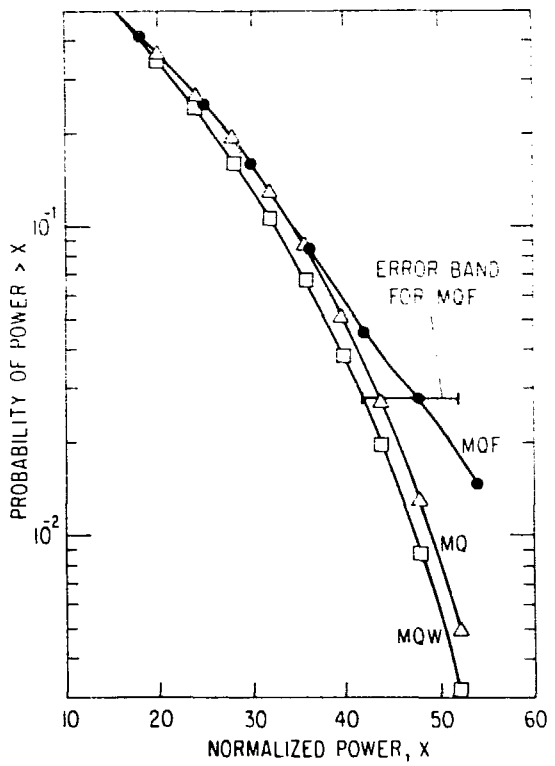

Fig. 3. Cumulative Distribution of the Normalized Reactor Power