CONF-870971--3

DE88 000585

CONF-870971--3

DETERMINISTIC METHODS FOR SENSITIVITY AND UNCERTAINTY ANALYSIS IN LARGE-SCALE COMPUTER MODELS*

B. A. Worley, E. M. Oblow, F. G. Pin, and R. E. Maerker

Engineering Physics and Mathematics Division
Oak Ridge National Laboratory
P.O. Box X
Oak Ridge, TN 37831-6364

J. E. Horwedel, R. Q. Wright, and J. L. Lucius

Computing and Telecommunications Division
Oak Ridge National Laboratory
P.O. Box X
Oak Ridge, TN 37831-6357

*Research sponsored by National High-Level Waste Management Program of the U.S. Department of Energy, under contract No. DE-AC05-84OR21400 with Martin Marietta Energy Systems, Inc.

ABSTRACT

The fields of sensitivity and uncertainty analysis have traditionally been dominated by statistical techniques when large-scale modeling codes are being analyzed. These methods are able to estimate sensitivities, generate response surfaces, and estimate response probability distributions given the input parameter probability distributions. Because the statistical methods are computationally costly, they are usually applied only to problems with relativively small parameter sets. Deterministic methods, on the other hand, are very efficient and can handle large data sets, but generally require simpler models because of the considerable programming effort required for their implementation. The first part of this paper reports on the development and availability of two systems, GRESS and ADGEN, that make use of computer calculus compilers to automate the implementation of deterministic sensitivity analysis capability into existing computer models. This automation removes the traditional limitation of deterministic sensitivity methods. The second part of the paper describes a deterministic uncertainty analysis method (DUA) that uses derivative information as a basis to propogate parameter probability distributions to obtain result probaability distributions. The last part of the paper demonstrates the deterministic approach to sensitivity and uncertainty analysis as applied to a sample problem that models the flow of water through a borehole. The sample problem is used as a basis to compare the cumulative distribution function of the flow rate as calculated by the standard statistical methods and the DUA method. The DUA method gives a more accurate result based upon only two model executions compared to fifty executions in the statistical case.

I. INTRODUCTION

The Office of Nuclear Waste Isolation (ONWI) is performing sensitivity and uncertainty studies as part of its performance assessment of a high-level nuclear waste repository in salt.[1,2] The role of the sensitivity analysis is to provide a means to limit the scope of the more complicated problem of quantifying uncertainties. Uncertainty analyses will be performed to support design reliability studies, to produce a cost-benefit analysis in conjunction with cost estimates, to insure compliance with regulatory criteria, and to help identify important research and development needs.

The sensitivity analysis of computer-generated results consists of determining the effect of model data upon the calculated results of interest. Because computer model equations can be differentiated analytically, sensitivities can be precisely defined and calculated in a deterministic fashion using both direct and adjoint methods.[3-10] The deterministic approach is particularly suited to large-scale problems for which direct perturbation of the model data becomes impractical from a cost standpoint. The main drawback to the deterministic approach has been the initial manpower investment to add the computational capability for calculating the necessary derivatives into existing computer models.

For quantification of uncertainties in computer-generated results, the problem can be expressed more precisely as the propagation of input uncertainties through models by the laws of probability to obtain output uncertainties. (The uncertainty associated with whether the computer model accurately reflects the physical phenomena is a problem of model validation and is not addressed in this paper.) Uncertainties of computer results are of primary interest in applications such as repository performance assessment in which experimental validation is not possible

or practical. Because of the complicated nature of the computational structure of large computer models, and because of the large number of input and data parameters associated with such models, to date almost all uncertainty analysis of computer results has been performed using a statistical approach.[11-14]

This paper presents a comprehensive approach to sensitivity and uncertainty analysis of large-scale computer models that is analytic (deterministic) in principle and that is firmly based on the model equations. The theory and application of two systems based upon computer calculus, GRESS [15,16] and ADGEN [17], are discussed relative to their role in calculating model derivatives and sensitivities without a prohibitive initial manpower investment. A Deterministic Uncertainty Analysis (DUA) method [18] that retains the characteristics of analytically computing result uncertainties based upon parameter probability distributions is then introduced. Finally, the role of sensitivity analysis and the DUA method are demonstrated on a sample problem describing the flow of water through a borehole.

II. DETERMINISTIC SENSITIVITY ANALYSIS

A brief description of general sensitivity theory is given here as an aid to understanding the problem of applying this theory to computer models. The example to be discussed will be that of a general set of non-linear equations given by

$$y = F(y,c) \quad , \tag{1}$$

where y represents the dependent variable being solved for, c represents the user-specified model data or parameter set, and F defines the model equations. The particular form chosen in Eq. (1) is one that can be used generally to represent equations coded in the FORTRAN programming language. The left side of the equation can represent the stored value of the variable calculated from the functional formula on the right side.

Since the number of components of the vector y calculated in any typical large-scale modeling problem is large, it is useful to define a generic result for such a calculation that is of particular interest to the model user. Typically many results will be needed for analysis but in most cases they form a much smaller set than the actual set of y component values. A typical result will be defined as

$$R = h(y) \quad , \tag{2}$$

where R is a single number that is a function of the solution to Eq. (1). For notational ease, the generic parameter α_i will be used to denote any individual parameter. The total number of parameters in the problem will be assumed to be M so that the index on α_i will run from 1 to M.

The basic problem in any sensitivity study is to find the rate of change in the result R arising from changes in any model parameters. For the generic parameter α_i, then, the quantity of interest is the numerical value of $dR/d\alpha_i$ given analytically by

$$\frac{dR}{d\alpha_i} = \frac{\partial h}{\partial y}\frac{dy}{d\alpha_i} \quad . \tag{3}$$

Since the functional dependence of R on y through h(y) is defined analytically by the model user, only $dy/d\alpha_i$ needs to be generated in order to evaluate Eq. (3). The procedure needed to get $dy/d\alpha_i$ is to differentiate Eq. (1) as follows:

$$\frac{dy}{d\alpha_i} = \frac{\partial F}{\partial y}\frac{dy}{d\alpha_i} + \frac{\partial F}{\partial c}\frac{dc}{d\alpha_i} \quad . \tag{4}$$

Rearranging Eq. (4) yields the following set of coupled equations to solve for $dy/d\alpha_i$,

$$\left(I - \frac{\partial F}{\partial y}\right)\frac{dy}{d\alpha_i} = \frac{\partial F}{\partial c}\frac{dc}{d\alpha_i} \quad , \tag{5}$$

or in more compact form,

$$Ay_i' = s_i \quad , \quad i = 1,\ldots,M \quad , \tag{6}$$

where I is the identity matrix and A, y_i', and s_i are given by

$$A = I - \frac{\partial F}{\partial y} \quad , \tag{7}$$

$$y_i' = \frac{dy}{d\alpha_i} \quad , \tag{8}$$

and

$$s_i = \frac{\partial F}{\partial c}\frac{dc}{d\alpha_i} \quad . \tag{9}$$

If Eq. (6) were solved directly for y_i', the result could be used in Eq. (3) to evaluate $dR/d\alpha_i$. This method of sensitivity analysis is called the "direct" approach and is a classical methodology that has received a great deal of attention in the literature.[3,7] Since Eq. (6) must be solved each time a new α_i is defined, the direct approach is most

suitable for problems with relatively few input parameters of interest, for problems in which the solution of Eq. (6) is very inexpensive compared to the solution of the model itself, or for analytical problems in which the inverse of A can be explicitly determined.

For large-scale models with a large data base in which the ultimate objective is still the evaluation of $dR/d\alpha_i$, the intermediary step of solving for $dy/d\alpha_i$ and its inherent computational inefficiency can be avoided. For such problems the "adjoint" approach is far more applicable. In this methodology, use is made of the fact that Eq. (6) is linear in y_i', and appropriate adjoint equations can therefore be developed specifically to evaluate Eq. (3).

Defining the matrix adjoint of A as A* and using the usual definition of this adjoint give the identity,

$$u^{tr}Av = v^{tr}A^*u \quad , \tag{10}$$

where u and v are arbitrary vectors and A* is defined as

$$A^* = A^{tr} \quad . \tag{11}$$

Here the tr superscript represents the transpose of the vector or matrix.

If specific vectors for the problem at hand are chosen for u and v, the problem-specific adjoint equation can be set up as follows:

$$A^*y^* = s^* \quad , \tag{12}$$

where

$$A^* = A^{tr} = \left(I - \frac{\partial F}{\partial y}\right)^{tr} \quad . \tag{13}$$

Choosing s* as

$$s^* = (dh/dy)^{tr} \quad , \tag{14}$$

Eq. (3) can now be evaluated as follows:

$$\frac{dR}{d\alpha_i} = y^{*tr} \frac{\partial F}{\partial c} \frac{dc}{d\alpha_i} \quad , \quad i = 1,\ldots,M, \tag{15}$$

where y* is now the solution to

$$\left(I - \frac{\partial F}{\partial y}\right)^{tr} y^* = \left(\frac{dh}{dy}\right)^{tr} \quad . \tag{16}$$

The simplicity of the adjoint approach lies in the fact that Eq. (16) needs to be solved only once to get any and all sensitivities in the problem. This is a result of Eq. (16) being independent of the definition of α_i. The particular choice of α_i is only reflected in the evaluation of Eq. (15), which involves simple vector products. In essence, the adjoint approach reduces the computational effort needed to evaluate $dR/d\alpha_i$ from solving many coupled linear equations to the evaluation of several vector products. For large-scale systems with many thousands or even millions of parameters, this represents orders of magnitude in computational efficiency.

It should be noted here that both the direct and adjoint equations (i.e., Eqs. (6) and (16)) are in any case far easier to solve than the original model (Eq. (1)). Both Eqs. (6) and (16) are linear while Eq. (1) is nonlinear. The direct and adjoint approaches, however, require the results of the original model equations to be available in order to set up Eqs. (6) and (16), since the A matrix and the vectors s, and s* depend on y.

In order to solve either the direct or adjoint sensitivity analysis, then, the model user must first generate the matrices $\partial F/\partial y$ and $\partial F/\partial c$

from the original nonlinear computer model. For large-scale problems this generally requires a great deal of painstaking human effort. First, the model equations must be extracted from the computer coding. They must then be differentiated with respect to all parameters of interest, and finally direct or adjoint sets of equations must be set up for computational solution. Successful automation of this procedure greatly reduces the human effort involved, potentially by orders of magnitude. The advantage of automation of sensitivity model development is therefore great indeed. The next two sections discuss two automated systems that use calculus precompilers to add capability to existing FORTRAN computer models for solving the direct and adjoint equations procedures.

III. GRESS

An Automated System for Solving the Direct Sensitivity Problem

For large-scale computer models, the equations are usually very complex and tied closely to and embedded in complex model logic and data-handling routines. In addition, for nonlinear problems, the numerical solution procedure often precludes an easy separation of the modeling equations from other parts of the model coding structure. For these reasons, a general system was developed to automate the application of computer calculus in existing codes. The system first developed for solving the direct sensitivity problem was the GRadient-Enhanced Software System (GRESS). Details of the GRESS system are given in Refs. 15 and 16, and the underlying ideas are briefly summarized herein.

The basic principle of GRESS is to read the model source program and search for model equations. These are identified uniquely by the

appearance in the FORTRAN source program of the "=" symbol. Since all FORTRAN "equations" so identified occur in the form of Eq. (1) (i.e., with a single dependent variable on the left side of such an expression), GRESS can search for and analyze each equation in terms of its functional dependence on y and c. The basic computer calculus operations of GRESS are then used to compute the successive elements of $\partial F/\partial c$ and $\partial F/\partial y$ as each expression is encountered. The differentiation is carried out analytically using calculus software for all permissible FORTRAN functions and operators and the results are computed and stored numerically using the local (current) values of the independent and dependent variables. GRESS takes advantage of the fact that in solving Eq. (5), the matrix $(I - \partial F/\partial y)$ is lower tridiagonal and the y vector can be computed by forward substitution. The important point is that the components of y are solved successively as each equation is differentiated and that the $(I - \partial F/\partial y)$ matrix does not have to be stored. (The adjoint problem requires the storage of this matrix, as will be discussed in the next section).

GRESS only recognizes real-variable store operations as valid equations (i.e., the left side variable in a FORTRAN equation must be real), since continuous derivatives are to be calculated. Also, the left hand side of an equation is treated as a separate component of y each time it is executed (including each execution in a DO LOOP). The calculation of $\partial F/\partial y$ and $\partial F/\partial c$ in effect means that GRESS can be used to calculate the derivative of any real variable in the model with respect to any other real variable in the model. All derivatives are available for both internal and/or external use. For example, the derivatives $dR/d\alpha_i$ are used in the DUA method to be described later.

The application of GRESS to an existing FORTRAN model is illustrated in Fig. 1. In the preliminary preprocessing step, the FORTRAN model is separated into two subsets. The first, which contains all main sequence computations, is hand modified for submission to the GRESS precompiler. The amount and nature of these modifications depend on the particular application at hand and the limitations of the current version of GRESS. GRESS presently recognizes all FORTRAN 77 functions with the exception of complex functions. The second subset (possibly null) is composed of subroutines whose only communication with the first subset is through the arguments in their calling sequence. These subroutines are usually associated with input, output, and peripheral program-analysis functions. They do not require GRESS compilation and may usually be submitted unchanged to the FORTRAN compiler.

The next step is the GRESS precompilation in which the automated code translation necessary to compute derivatives is performed using automated computer calculus. This step consists primarily of a rearrangement of the program data structure and a substitution of calls to GRESS interpretive software in place of all arithmetic lines of coding. All arithmetic operations of the original model are precompiled into a pseudomachine code (the GRESS P-code) for use during program execution. The two output files of this step are the enhanced model and the binary P-code file. These two files and a set of GRESS software subroutines supporting the enhanced model are compiled and run as a normal FORTRAN program to produce both the reference model results and gradient information. The gradients and reference results are used to calculate the sensitivities.

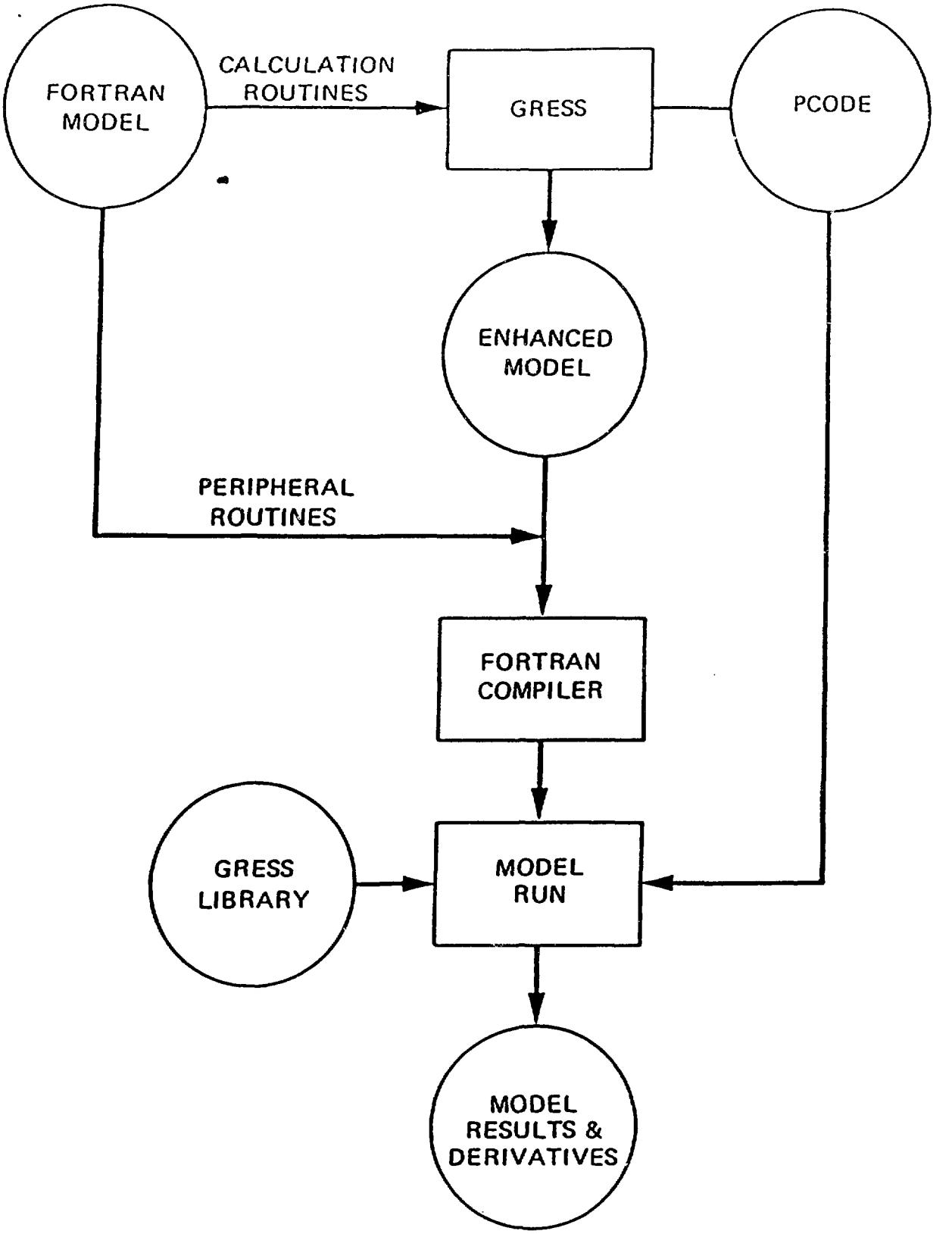

Figure 1 - GRESS Flowchart

GRESS has undergone extensive verification during its development. To date, five major computer models of interest to ONWI have been enhanced using GRESS, with direct comparison of GRESS-calculated derivatives to perturbation-derived derivatives being made for each enhanced model.[19-23]

IV. ADGEN

An Automated System for Solving the Adoint Sensitivity Problem

The adjoint problem is defined by Eqs. (12-16). As previously mentioned, the calculation of the adjoint solution vector y^* from Eq. (16) is not a function of the selection of input parameter α_i and thus need only be performed once to determine the derivatives of a response of interest with respect to any parameter of interest. The matrix $\partial F/\partial c$ must also be determined but it too is independent of the parameter of interest. The only parameter dependent operation required to calculate the derivative $dR/d\alpha_i$ is the simple matrix multiplication operation $(y^{*tr})(\partial F/\partial c)(dc/d\alpha_i)$ in which the vector $dc/d\alpha_i$ is a function of α_i. A system to automate the calculation of derivatives based upon the solution of the adjoint equations has been developed.[17] The system is named ADGEN (ADjoint GENerator) and uses a GRESS-like precompiler named EXAP (Extended Arithmetic Processor) which will enhance any FORTRAN code with the computer calculus necessary to calculate all required derivatives of the $\partial F/\partial y$ and $\partial F/\partial c$ matrices.

Recall that GRESS solves Eq. (5), taking advantage of the fact that the matrix $(I - \partial F/\partial y)$ is lower tridiagonal and the solution by forward substitution requires only that the vector $dy/d\alpha$ be stored. However, to

solve the adjoint problem, the EXAP precompiler must calculate and store all derivatives that constitute the n x n matrix $(I - \partial F/\partial c)^{tr}$, where n = total number of equations, counting each time an equation is solved in a DO LOOP as a separate equation; the left hand side of each equation in a DO LOOP is treated as a separate element of y. Although only the non-zero elements are saved, the storage of the matrix $(I - \partial F/\partial c)^{tr}$ may require a substantial amount of storage capability. The storage difficulties are counterbalanced by features of Eqs. (15) and (16) that make the ADGEN calculation of y* both practical and cost efficient. Note that the matrix $(I - \partial F/\partial c)^{tr}$ is upper tridiagonal and that the column vector $(dh/dy)^{tr}$ is a simple user-defined vector (for most cases a vector with a single non-zero entry of unity). Thus Eq. (16) is easily solved by back substitution and the values of y^* can be successively stored in the space allocated for the $(dh/dy)^{tr}$ vector. The calculation of $dR/d\alpha_i$ from Eq. (15) must be performed for each α_i but this requires only trivial matrix multiplications and very little computer cost.

The ADGEN system is shown schematically in Fig. 2. Like GRESS, the ADGEN precompiler EXAP produces a binary file that essentially contains all the arithmetic operations of the code being enhanced. The enhanced code has CALL statements that access the P-CODE and calculates the normal model results as well as the derivatives making up the $\partial F/\partial y$ and $\partial F/\partial c$ matrices. One major difference from the GRESS schematic (Fig. 1) is the requirement to store the $(I - \partial F/\partial c)^{tr}$ matrix and the need for a post-processor solver routine to calculate the adjoint solution.

The testing and verification of ADGEN has been performed on the PRESTO-II computer model [24], which has approximately 6,900 lines of

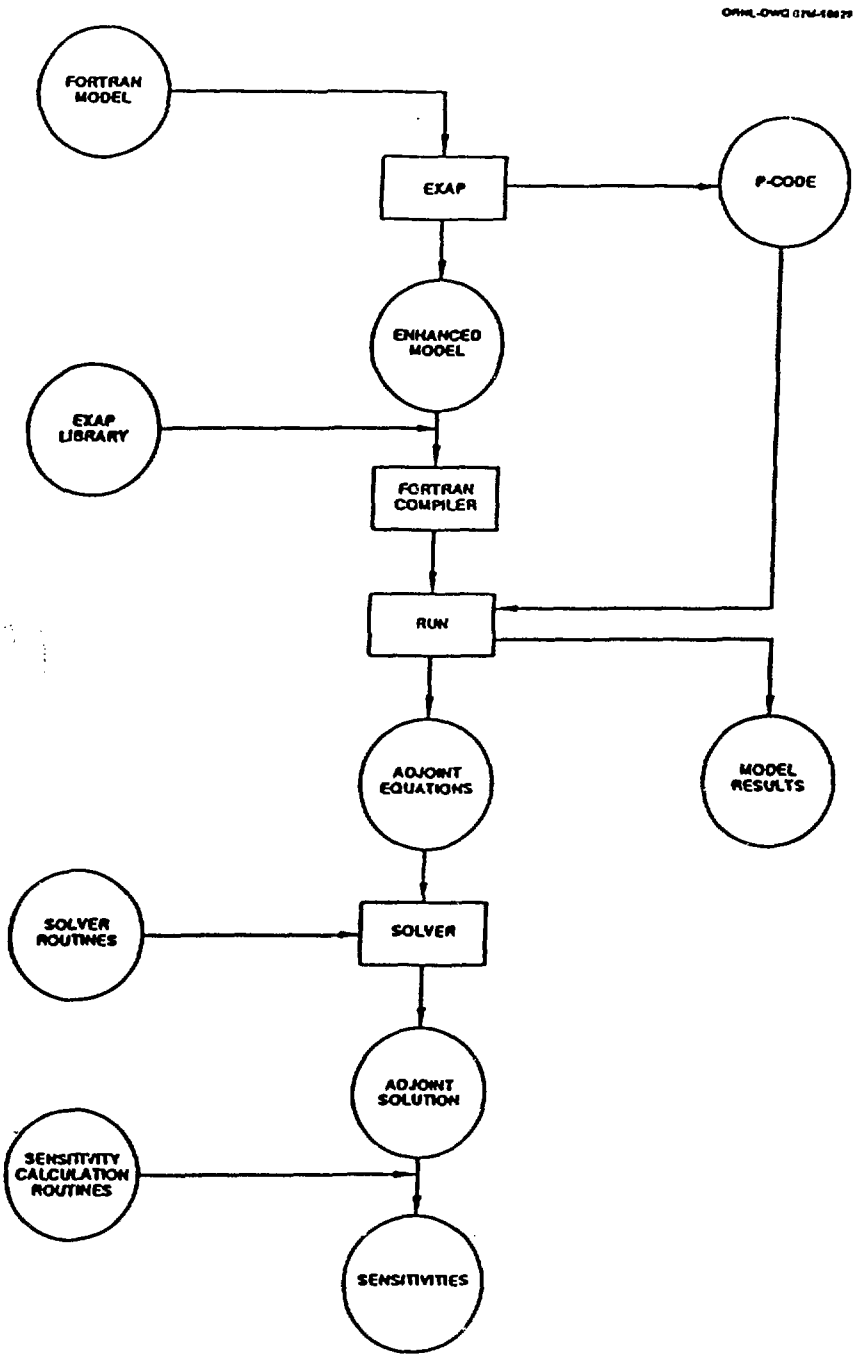

Figure 2 - ADGEN Flowchart

coding. The sample problem included in Ref. 24 calculates a time-dependent radiation dose to man from transport of 42 radionuclides. The problem has a large data base of approximately 69,000 input parameters. ADGEN was used to calculate the derivatives of the dose to all 69,000 parameters and direct perturbation was used to verify selected derivatives. For this problem the $(I - \partial F/\partial y)^{tr}$ matrix had approximately 870,000 rows, requiring about 19,700 Kbytes of memory.

V. DETERMINISTIC UNCERTAINTY ANALYSIS

The analytical propagation of input uncertainties through a calculational model is unfeasible, if not impossible, for all but the most simple models. The difficulty lies in mapping probability density functions from an M-dimensional space of input parameters to the singly dimensioned output distribution function. To circumvent this problem, the most common approach is to randomly sample the input distributions and then calculate the model output of interest, constructing a probability distribution of the output by rerunning the model for each sample set of input parameters. The input probability distributions and any parameter correlations are handled, in a statistical sense, in the sampling procedure.[13,14] The information available from probability propagation is lost, but hopefully the sampling procedure will lead to an output distribution that is representative of that which would result from the actual propagation of input probability distributions. As the number of sampling sets increases, the difference between the calculated and "true" output distribution diminishes. The problems occur in practice when the number of runs of the computer model needed to assure a large enough statistical sample becomes too expensive.

Another approach is to discretize the input probabilities into histograms and evaluate the model output of interest for all possibilities of parameter combinations to form a probability tree.[25] All parameter correlations are incorporated into the probability tree structure. This method does not rely on random sampling and probabilities are easily propagated in probability trees by simple multiplication. The histogram probability distributions are not actually propagated, but rather mean or endpoint parameter values are used. This method is quite feasible for models with a small number of parameters or even for a large number of input parameters if the model is simple (inexpensive). Again the problem arises when the computer model has numerous input parameters and/or is expensive to run.

A third approach is the response surface method in which the computer model is replaced with a simple analytical expression.[26] The expression is constructed by fitting the computed values of the model output to the corresponding input parameters, or more generally, to chosen functions of the input parameters. The uncertainty in the computed value of the expression is then determined in the usual statistical sense by sampling of the input distributions. The advantage of replacing the model with the response surface is the drastically reduced computational time to compute the expression result compared to running the computer model. The disadvantage is the introduction of error in the calculated output by replacement of the model with a simple expression.

The Deterministic Uncertainty Analysis (DUA) method [18] combines the characteristics of the response surface method and probability trees. Statistical sampling is not required and probabilities are propagated analytically within discretized numerical meshes that encompass the

parameter space. The approach underlying the deterministic calculation of uncertainties in the DUA method relies upon (1) a replacement of the computer model with an analytical function relating the responses of interest to the parameters of interest and (2) discretizing the parameter space and calculating the expected value of the response within each discrete parameter space "mesh." The parameters of interest are chosen to be those that are "uncertain," meaning that they have known or assumed probability distributions. The parameters of interest may often include the entire set of data used by the computer model.

This deterministic approach differs from the response surface methods in two ways. First, the analytical function is constructed based upon the response value of interest as well as the partial derivatives of the response with respect to each of the parameters. The classical response surface method constructs the surface (analytical expression) based only upon the response value at each parameter space point. Thus the degrees of freedom with which to fit the response to the parameter values is much greater in the DUA method than in the response surface methods. There is of course no reason to distinguish this aspect of the DUA method from response surface methods if the response surfaces are constructed using derivative data; but in the classical response surface methods these derivatives are assumed to be unavailable, most likely since the response surface methods grew out of experimental design fields in which only set points of the control variables (parameters in our terminology) and the experimental measured values (responses) are known. As the response surface methods came to be used for replacement of large, complex computer models, again the derivative information was not used because of the difficulty of calculating partial derivatives chained

through complex computational paths. However, the development of efficient methods for calculating derivatives and sensitivities for large-scale computer model results has progressed steadily based upon a firm theoretical foundation. Moreover, with the availability of GRESS and ADGEN, the calculation of derivative information for the purpose of improving the formation of response surfaces is both practical and cost effective. This availability of derivative information is a key component in the DUA method.

The second feature that distinguishes the DUA method from response surface methods, and a feature that it has in common with probability tree methods, is that the entire parameter space is spanned. In the response surface methods, the construction of response surfaces has been primarily used to dramatically increase the number of sampling points in a statistical determination of response probability distributions since the evaluation of the analytical response surface expression is much less expensive to obtain than the corresponding computer model result. However, only by spanning the entire parameter space can probabilities be propagated, either through a computer model or through an analytical expression. Spanning the entire parameter space is practical only if the discretization of parameter probability distributions is performed over a reasonably large mesh. In probability tree methods, for example, the probability distributions are typically replaced with the high and low values of the distribution. The DUA method extends the probability tree methods into a more rigorous propagation of probabilities in two ways: (1) Since an analytical expression relates the response to the parameters, the expected value of the response over each discretized mesh can be calculated analytically and thus gives a more meaningful value than just a single sampling point within the mesh. (2) Because the computer

model is replaced with an analytical expression, a finer mesh size can be constructed over the parameter space and a more accurate representation of the parameter probability distributions of most interest can be obtained.

Another point to be made in favor of propagating probabilities through an expression that can only approximate the original computer model, and one that makes the DUA method possible for computer models with a large number of parameters, is the integral nature of the probability distribution of the response. The probability distribution of the response of interest is an integral quantity and errors introduced by replacement of the computer model with an analytical expression are most often washed out when the parameter space is completely spanned.

Formation of Response Surface Using Derivative Information

The DUA method replaces the computer model with a response surface by relating the response of interest as calculated by the computer model to the parameter values by techniques that incorporate knowledge of the partial derivatives of the response with respect to the parameters of interest. The simplest form of a response surface is one formed by linear extrapolation from reference space points to each mesh of the discretized parameter space. Within each mesh the response surface is linear with respect to the parameters, and the calculation of the expected value of the response within the mesh, given parameter probability functions, is straightforward. An extrapolation scheme that makes use of the sensitivities is outlined in Ref. 18.

A more general approach for construction of a response surface is a least-squares fitting technique. Possible schemes for incorporating

derivative information into the standard fitting technique are presented in Ref. 18. Basically, to construct a response surface to a given order of expansion, the use of derivative information reduces the number of computer runs required to uniquely determine the expansion coefficients by a factor of approximately 1/M, where M is the number of parameters. One can either construct a global response surface or define local response surfaces over subregions of the parameter space. A local fit of the response values and derivatives using a low-order function may be more desirable than a global fit using a higher order function to fit a large portion of the data because a higher order fit involving many response points may result in a very radically behaved function in the parameter space not near the fitted points. For this reason most of our research to date has focused upon either local fitting or linear extrapolation from reference parameter space points. By careful selection of these parameter space points for which model results will be obtained (using Latin Hypercube Sampling, for example), the number of computer runs can be held to a small fraction ($<< 1/M$) of the number required for the conventional construction of a response surface.

Finally, sensitivity analysis plays an important role in the formation of the response surface by eliminating those parameters that have a negligible effect on the result of interest based on their sensitivities and uncertianty ranges. Also, the derivative information from the reference model runs can be used to identify the occurence of parameters that occur exclusively in a given combination. Such identification reduces the parameter space by replacement of the individual parameters with the particular combination. For example, if the derivative of the response with respect to each of two paramters is the same at each reference space

point sampled, the two parameters most likely appear in the model as a sum of each other, and a single parameter representing the sum of the two can be used in the formation of the response surface in place of the two individual parameters. The sample problem exemplifies these uses of sensitivity and derivative data in the formation of the response surface.

Propagation of Probabilities

The propagation of parameter probability distributions from the multidimensional parameter space to the singly dimensioned result space is determined by the governing system of equations and the input variable probability density functions (pdf's). In theory this propagation can be performed analytically by convolution of the integral of the parameter space into a discrete number of integrals of the singly-dimensioned response space, in which each integral is over a monotonically changing function representing the result. However, because the identification of the convolution integrals, in particular the limits of the integrals, is virtually impossible for all but the simplest problems, and because the model equations are nonlinear and complexly intertwined in general, the propagation of probability distributions through computer model cannot be treated analytically in the strictest sense.

The propagation of parameter probability distributions in the DUA approach is performed by discretizing the M-dimensional parameter space (M = number of parameters) into L meshes, each mesh denoted by m_ℓ. The probability of mesh m_ℓ occurring within the entire parameter space, $p(m_\ell)$, is calculated as well as the expected value of the response function within the mesh, $E(R_\ell)$, where R_ℓ represents the response function

within m_ℓ. The probability $p(m_\ell)$ is assigned to $E(R_\ell)$ to obtain the probability of $E(R_\ell)$ within the discrete space of expected values. The pairs of $p(m_\ell)$ and $E(R_\ell)$ are reordered such that $E(R_1) < E(R_2) < \ldots E(R_L)$ and as such constitute the probability density function of the response R over the parameter space. The cumulative distribution function (CDF) of R, C(R), is the running sum of the reordered $p(m_\ell)$ paired with the corresponding value of $E(R_\ell)$. In the limit as $L \Rightarrow \infty$, C(R) approaches the true cumulative distribution function of R as calculated using the response function.

Let the functional form of the response within m_ℓ be given by

$$R_\ell = g_\ell(c) \tag{17}$$

where $g_\ell(c)$ is the response surface function within m_ℓ resulting either from a fitting procedure or from a linear expansion from one or more reference space points. The vector c is the M-dimensional parameter vector given by $c = (\alpha_1, \alpha_2, \ldots, \alpha_M)_{tr}$. Given the joint probability function of c as $P(c) = P(\alpha_1, \alpha_2, \ldots \alpha_M)$, the probability that $c \subset m_\ell$ is given by

$$P(m_\ell) = P(c \subset m_\ell) = \int_{m_\ell} P(c)dc \quad , \tag{18}$$

and the expected value of the response R within m_ℓ, $E(R_\ell)$, is

$$E(R_\ell) = \int_{m_\ell} g(c)P(c)dc/p(m_\ell) \quad . \tag{19}$$

The values of $p(m_\ell)$ and $E(R_\ell)$ as calculated by Eqs. (18) and (19) are used to construct the probability density function and cumulative distributions function of the response R.

VI. SAMPLE PROBLEM

Reference 27 describes a sample problem that exemplifies the use of uncertainty-analysis in high-level waste applications. The sample problem consists of three coupled equations with eight input parameters and three dependent variables. The analysis focuses on one of the three dependent variables, the flow rate, as the response of interest, and statistical techniques are used to calculate the cumulative distribution of the flow rate given probability distributions for the eight input parameters.

The governing equations describe the downward flow of water through a borehole that is drilled from the ground surface through two aquifers. For a fully penetrating well and no ground-water gradient, the steady-state flow through the upper aquifer into a borehole is given by

$$Q = \frac{2\pi\ (H_u - H_{uw})\ T_u}{\ell n\ (r/r_w)} \tag{20}$$

where Q = flow, m^3/yr

T_u=transmissivity of upper aquifer, m^2/yr

H_u = potentiometric head of upper aquifer, m

H_{uw} = steady-state potentiometric head in borehole at upper aquifer, m

r = radius of influence, m

r_w = radius of borehole, m.

Similarly, the steady-state flow from the borehole to the lower aquifer is given by

$$Q = \frac{-\ 2\pi\ (H_\ell - Hw_\ell)\ T_\ell}{\ell n\ (r/r_w)} \tag{21}$$

where T_ℓ = transmissivity of lower aquifer, m^2/yr

H_ℓ = potentiometric head of lower aquifer, m

$H_{w\ell}$ = steady-state potentiometric head in borehole at lower aquifer, m.

The flow of water through the borehole is assumed to be laminar and isothermal and is given by

$$Q = \frac{\pi r_w^2 \, (H_{wu} - H_{w\ell}) \, K_w}{L} \tag{22}$$

where K_w = hydraulic conductivity of borehole, m/yr

L = length of borehole, m.

In Eqs. (20-22), Q, H_{wu}, and $H_{w\ell}$ are dependent variables; the flow rate of water, Q, is the response of interest. The uncertainty problem is to calculate the cumulative distribution function of Q, C(Q), given the probability density functions of the eight input parameters r_w, r, T_u, T_ℓ, H_u, H_ℓ, K_w, and L. The probability density functions of these eight parameters are given in Ref. 27.

The standard statistical approach for calculating C(Q) is to define a design matrix based upon the pdf's of the parameters. Several sampling procedures are available for determining a suitable design matrix. For this problem, Ref. 27 investigates the formation of design matrices based upon the Latin Hypercube Sampling (LHS) procedure using 10 and 50 design points. The choice of the sets of input parameters in a design matrix hopefully removes as much bias as possible from the selection procedure such that each calculated value of the response is of equal probability. Thus, the probability of a calculated response is 1/N, where N is the number of input sets in the design matrix and formation of C(Q) is

performed by ranking the values of Q from lowest to highest and apportioning a probability of 1/N to each value. Figure 3 shows the plots of C(Q) resulting from the use of the 10-point and 50-point LHS design matrices. Clearly, the 10-point LHS design matrix does not result in a curve for C(Q) that closely matches that of the 50-point set. It is important to keep in mind that a design matrix based on N input sets requires that the computer model be run N times to determine C(Q). For this sample problem, the "computer model" consists of Eqs. (20-22) and these were solved 10 times for the 10-point design matrix and 50 times for the 50-point design matrix.

Deterministic Sensitivity and Uncertainty Analysis of the Sample Problem

The DUA method was applied to this sample problem and the results compared to the published statistical results in Ref. 27. The choice of N reference points from which the response surface is formed in the application of DUA to this problem was chosen to be a subset of the 10-point LHS design matrix. For each reference point i, i=1,...,N, defined by the 8-dimensional parameter vector $c_i = (r_w^i , r^i , T_u^i , T_\ell^i , H_u^i , H_\ell^i , K_w^i , L^i)^{tr}$, the derivative vector $dR/dc = (\partial Q/\partial r_w)_i , (\partial Q/\partial r)_i , (\partial Q/\partial T_u)_i , \partial Q/\partial T_\ell)_i , (\partial Q/\partial H_u)_i , (\partial Q/\partial H_\ell) , (\partial Q/\partial K_w)_i , (\partial Q/\alpha L)_i)^{tr}$, and the response $Q(c_i)$ were calculated deterministically. Sensitivities of Q with respect to each parameter, defined by $(\alpha_k/Q(c)_i(\partial Q/\partial \alpha_k)_i$ were also computed. Parameters with sensitivities and uncertainty ranges such that their influence on Q was negligible were dropped from the parameter space for the purpose of forming the response surface. As a result, the parameters T_u, r, and T_ℓ were not used in the formation of the response

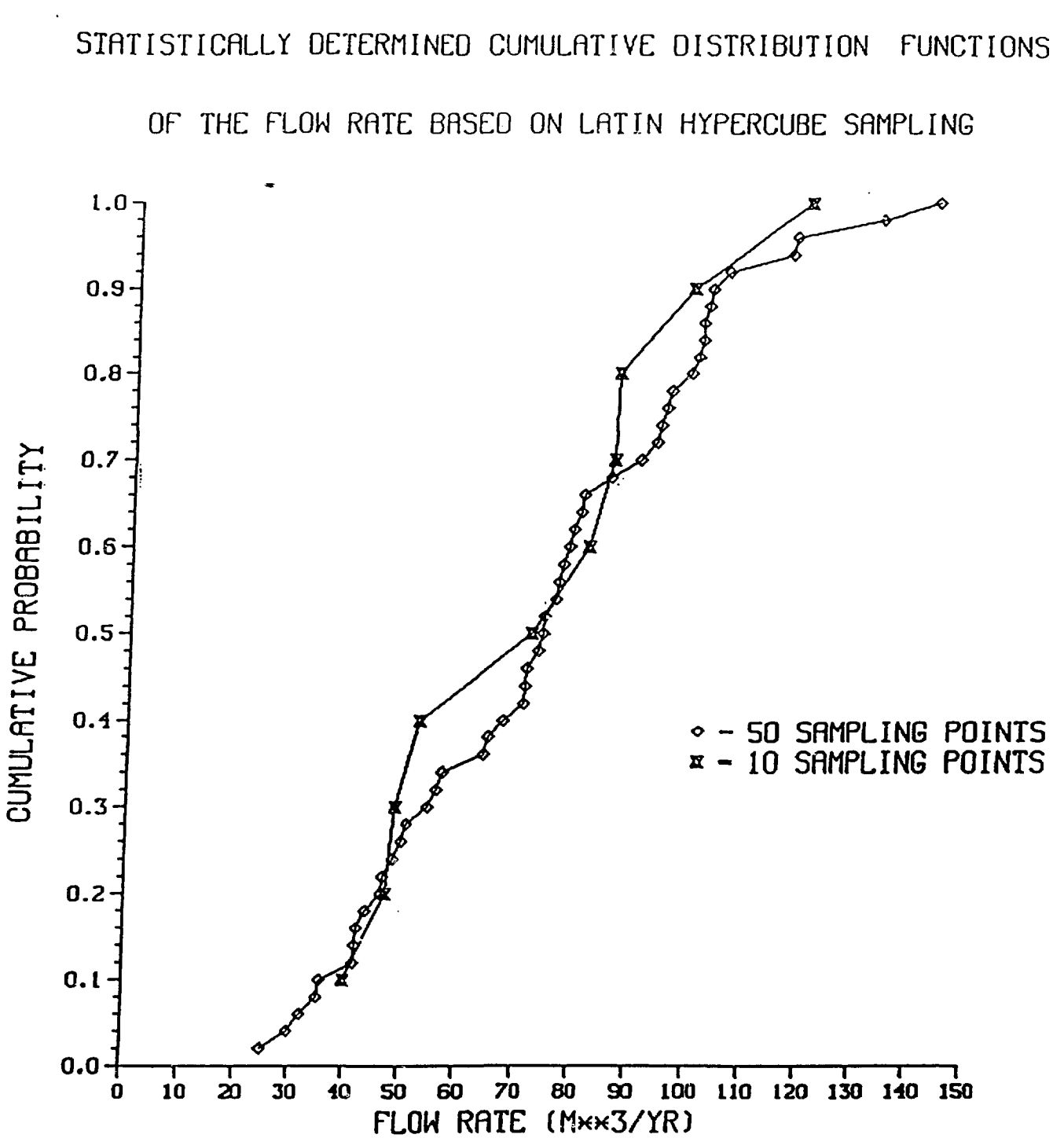

Figure 3 - CDF from 10-point and 50-point LHS design matrices.

surface. In addition, the derivatives of H_u and H_ℓ are equal but opposite in sign indicating that the two parameters occur in the model in the combination of $-(H_u-H_\ell)$. Therefore these two parameters were replaced by the single parameter (H_u-H_ℓ). The response surface was then constructed based on only the four significant parameters (H_u-H_ℓ), r_w, K_w, and L. This reduction in the number of significant parameters and combination of parameters illustrates the role of sensitivity analysis in the DUA method as applied to this sample problem.

In this application, the response surface was formed by linear extrapolations of Q from the reference points. The entire parameter space of significant parameters as identified in the sensitivity analysis (r_w, H_u-H_ℓ, K_w, and L) was divided into L discrete, nonoverlapping meshes, m_ℓ, $\ell=1,,,L$. The expected value of Q within each mesh, $E(Q_\ell)$, was determined by replacing Q_ℓ for g(c) in Eq. (19). Here, $Q_\ell = Q(c)$, $c \subset m_\ell$, where within m_ℓ, Q(c) was calculated by extrapolation. The mesh probability $p(m_\ell)$ was calculated from Eq. (13) using the parameter probability distributions from Ref. 27 ($p(H_u-H_l)$ had to be calculated separately using the individual distributions). The probability assigned to each $E(Q_\ell)$, $\ell=1,,,L$, was the corresponding value of $p(m_\ell)$. As discussed earlier, in the DUA method the number of meshes, L, is chosen such that the entire reduced parameter space is covered by nonoverlapping discrete meshes and therefore the entire probability space is complete.

As a benchmark against which a comparison of the DUA method and the statistical results from Ref. 27 could be compared, the sample problem model was executed 2304 times in order to approximate the "true" CDF of Q for this problem. A comparison of this benchmark 2304-point CDF to the

statistical 50-point CDF from Ref. 27 is shown in Fig. 4. The CDF based upon the 50 point LHS design matrix is a fairly accurate represention of the true CDF of Q. DUA method results were obtained by forming a response surface by extrapolation from two reference model runs and propogating parameter pdf's over a discrete mesh consising of 2304 meshes. As shown in Fig. 5., the CDF of Q calculated deterministically based on the DUA method closely matches the "true" CDF with only two executions of the derivative-enhanced model.

VIII. CONCLUSIONS

A comprehensive, deterministic approach to sensitivity and uncertainty analysis of large-scale computer models is now available. The GRESS and EXAP systems for automating the calculation of model derivatives and sensitivities have been developed, verified, and applied to several large-scale computer models. The availability of these two systems greatly reduces the man-effort required to add sensitivity capability to existing FORTRAN models.

A deterministic approach to uncertainty analysis (DUA) has been developed, and the availability of derivative information is a key component. The feasibility of the DUA method was verified by its application to a sample problem previously analyzed using a statistical approach. The sample problem results show that simple linear extrapolation from two space points produces a CDF of the response of interest that more closely matches a benchmark 2304-point CDF than does the CDF based upon a 50-point LHS design matrix. The reduction in model runs by a factor of 25 and the increased accuracy in calculating the CDF of the reponse of interest is strong evidence that a substantial savings in

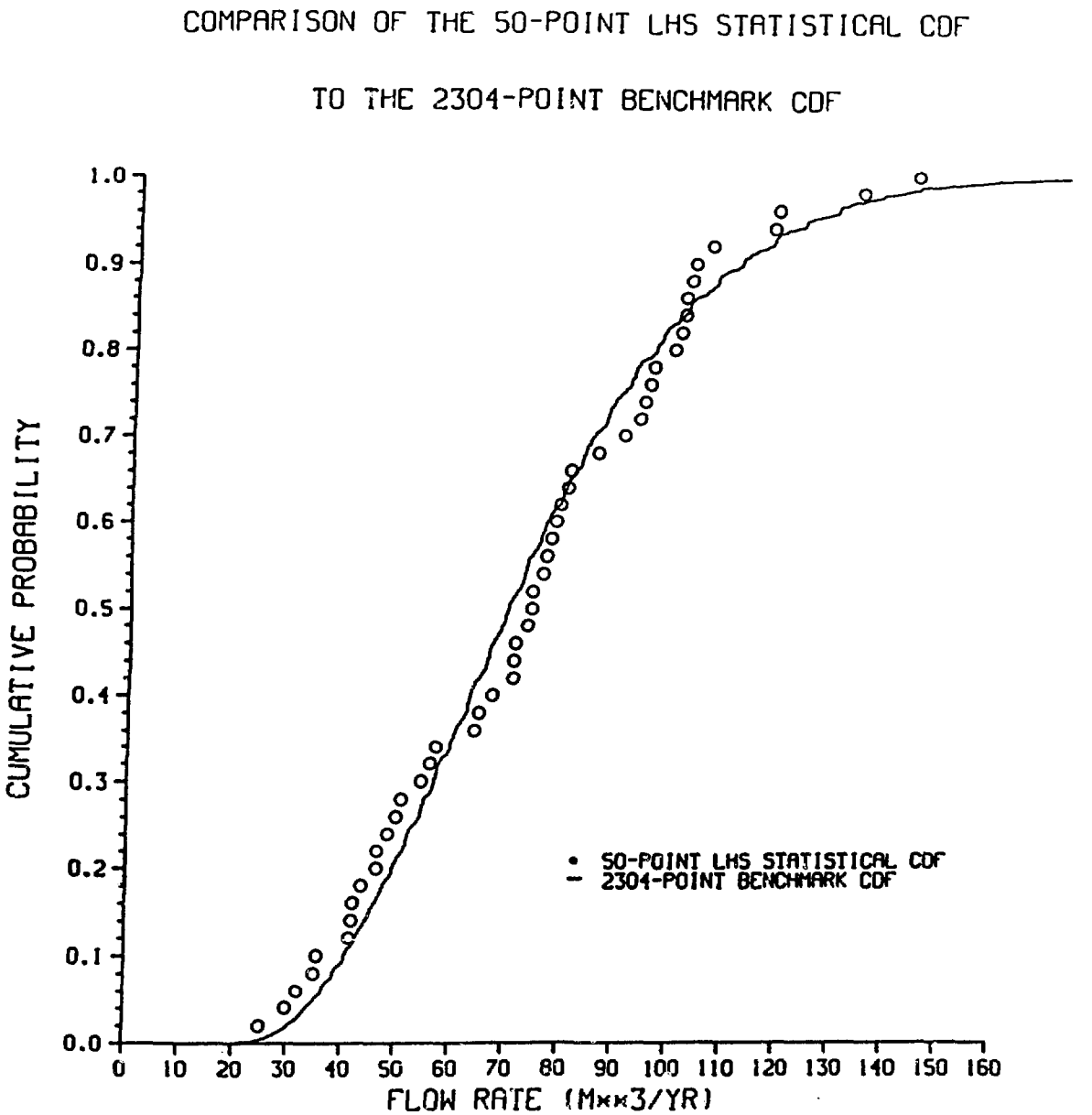

Figure 4 - 50-Point LHS CDF vs Benchmark CDF

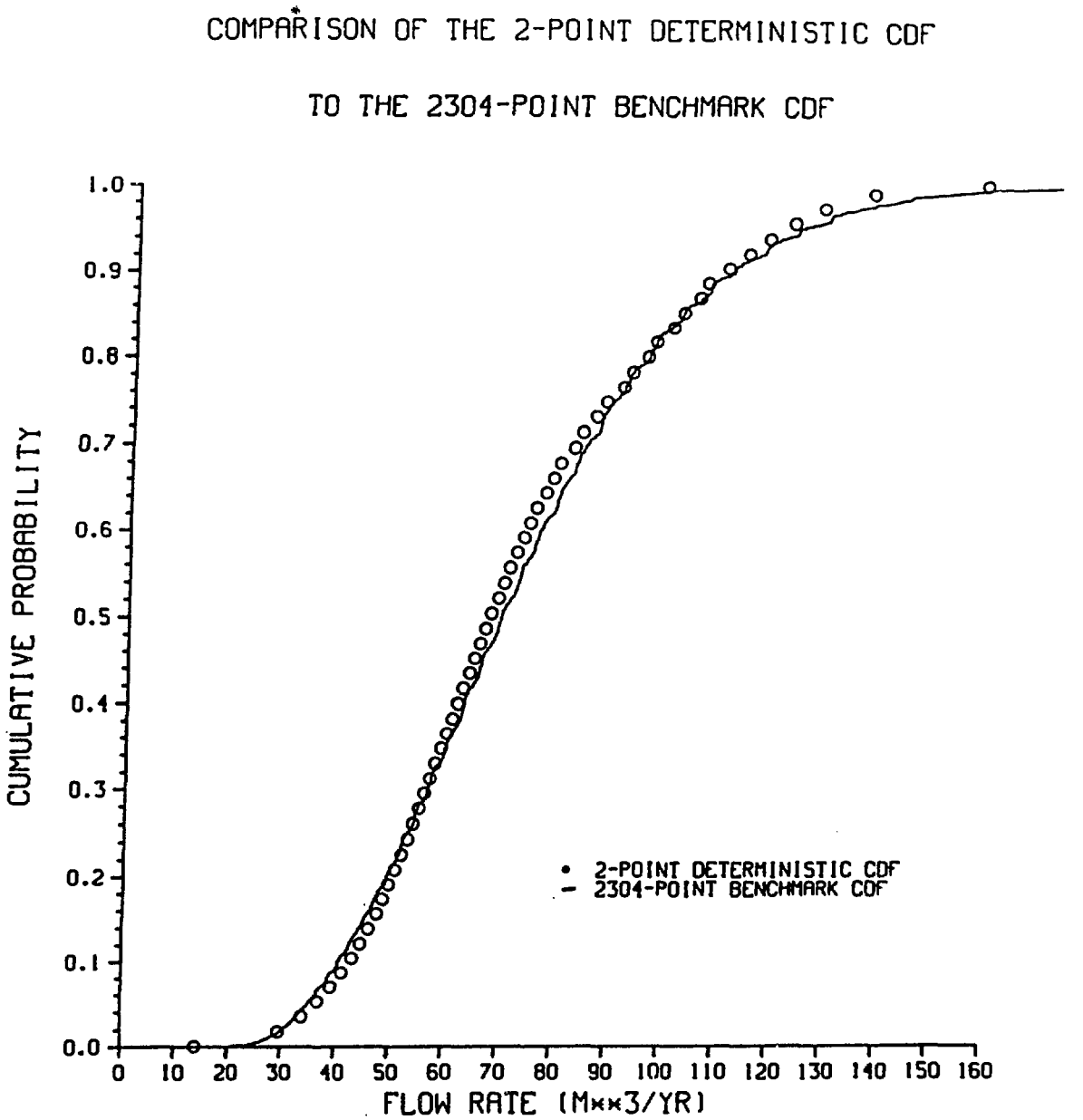

Figure 5 - Two-Point DUA CDF vs Benchmark CDF

computational cost is possible. This reduction is offset by the additional cost of calculating derivatives, but the deterministic calculation of model derivatives has been shown in the published literature to be both feasible and fairly cost efficient - certainly much less than a factor of 25. The availability of the GRESS and EXAP systems for adding derivative-taking capability to existing models makes the DUA approach even more practical. The strong analytical foundations of propagating probabilities deterministically is another desirable feature of the DUA approach.

PUBLICATIONS CITED

1. Thomas, R. E., "Uncertainty Analysis," ONWI-380, Office of Nuclear Waste Isolation, Battelle Memorial Institute, Columbus, Ohio (1982).

2. Harper, W. V., "Sensitivity/Uncertainty Analysis Techniques for Nonstochastic Computer Codes," ONWI-444, Office of Nuclear Waste Isolation, Battelle Memorial Institute, Columbus, Ohio (1983).

3. Tomovic, R. and Vukobratovic, M., **General Sensitivity Theory**, Elsevier North-Holland, Inc., New York (1972).

4. Stacey, W. M., **Variational Methods in Nuclear Reactor Physics**, Academic Press, New York (1974).

5. Greenspan, E., "Developments in Perturbation Theory," **Advances in Nuclear Science and Technology**, Vol. 9, Academic Press, New York (1976).

6. Oblow, E. M., **Nucl. Sci. Eng.**, 68, 332 (1978).

7. Frank, P. M., **Introduction to System Sensitivity Theory**, Academic Press, New York (1978).

8. Cacuci, D. G., **J. Math. Phys.** (NY), 22, 2794 (1981).

9. Cacuci, D. G., **J. Math. Phys.** (NY), 22, 2803 (1981).

10. Weisbin, C. R. et al, "Sensitivity and Uncertainty Analysis of Reactor Performance Parameters," **Advances in Nuclear Science and Technology**, Vol. 14, Plenum Press, New York (1982).

11. McKay, M. D., R. J. Beckman and W. J. Conover, **Technometrics**, 21, 239-245 (1979).

12. Iman, R. L., J. C. Helton, and J. E. Campbell, **J. Quality Technol.**, 13, 3, 174 (1981).

13. Iman, R. L., J. C. Helton, and J. E. Campbell, **J. Quality Technol.**, 13, 4, 232 (1981).

14. Iman, R. L., and Conover, W. J., "A Distribution-Free Approach to Inducing Rank Correlation Among Input Variables," **Communications in Statistics**, B11(3), 311-334, 1982.

15. Oblow, E. M., "An Automated Procedure for Sensitivity Analysis Using Computer Calculus," ORNL/TM-8776, Oak Ridge National Laboratory, Oak Ridge, Tennessee, 1983.

16. Oblow, E. M., "GRESS, Gradient-Enhanced Software System," ORNL/TM-9658, Oak Ridge National Laboratory, Oak Ridge, Tennessee, 1985.

17. Pin, F. G., Oblow, E. M., Horwedel, J. E., and Lucius, J. L., "ADGEN: An Automated Adjoint Code Generator for Large-Scale Sensitivity Analysis," paper to be presented at Am. Nuc. Soc. Winter Mtg., Los Angeles, California, Nov. 1987.

18. Worley, B. A., "Deterministic Uncertainy Analysis," ORNL-6428, Oak Ridge National Laboratory (1987).

19. Oblow, E. M., F. G. Pin, R. Q. Wright, **Nucl. Sci. Eng.**, **94**, 46 (1986).

20. Worley, B. A., R. Q. Wright, F. G. Pin, W. V. Harper, **Nucl. Sci. Eng.**, **94**, 180 (1986).

21. Pin, F. G., B. A. Worley, E. M. Oblow, R. Q. Wright, W. V. Harper, **Nucl. and Chem. Waste Man.**, **6**, 255 (1986).

22. Worley, B. A., R. Q. Wright, F. G. Pin, "A Finite-Line Heat Transfer Code with Automated Sensitivity-Calculation Capability," ORNL/TM-9975, Oak Ridge, Tennessee (1986).

23. Worley, B. A., J. E. Horwedel, "A Waste Package Performance Assessment Code with Automated Sensitivity-Calculation Capability," ORNL/TM-9976, Oak Ridge, Tennessee (1986).

24. Fields, D. E., et al., "PRESTO-II: A Low-Level Waste Environmental Transport and Risk Assessment Code," ORNL-5970, Oak Ridge National Laboratory, Oak Ridge, TN (1986).

25. Sutcliffe, W. G., "Uncertainty Analysis: An Illustration from Nuclear Waste Package Development," **Nucl. and Chem. Waste Manag.**, 5, 131 (1984).

26. Myers, R. H., **Response Surface Methodology**, Allyn and Bacon, Inc., Boston, Massachusetts, 1971.

27. Harper, W. V., and Gupta, S. K., "Sensitivity/Uncertainty Analysis of a Borehole Scenario Comparing Latin Hypercube Sampling and Deterministic Sensitivity Approaches," BMI/ONWI-516, Office of Nuclear Waste Isolation, Battelle Memorial Institute, Columbus, Ohio, 1983.