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# Development of Statistical Package for Uncertainty and Sensitivity Analysis(SPUSA) and Application to High Level Waste Repostitory System

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# 불확실도와 민감도 분석용 통계 패키지(SPUSA)개발 및 고준위 방사성 폐기물 처분 계통에의 응용

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## Abstract

For the probabilistic risk assessment of the high level radioactive waste repository, some methods have been proposed up to now. Since the system has highly uncertain input parameters, the evaluated risk for some input parameter values has high uncertainty. In this paper, methods of uncertainty and sensitivity analysis are devised to analyze systematically these factors and applied to a probabilistic risk assessment model of the high level waste repository.

The statistical package SPUSA developed through this study can be used for any other fields, e.g., statistical thermal margin analysis, source term uncertainty analysis, etc.

## 요 약

고준위 방사성폐기물 처분장에 대한 확률론적 위험도 평가를 위해 지금까지 많은 방법들이 제안되어 왔다. 이 계는 많은 불확실성을 갖는 입력 변수들을 갖고 있어서 이 입력변수들에 대해 계산된 위험도 역시 많은 불확실성을 갖는다. 본 논문에서는 이러한 점들을 조직적으로 분석하기 위하여 여러가지 불확실도 및 민감도 분석 방법들이 개발되었고 고준위 폐기물 처분장의 위험도 평가에 적용되었다.

본 논문을 통해 개발된 통계 패키지 SPUSA는 통계적 열여유도 분석, 방사선원 불확실도 분석등등의 분야에도 사용될 수 있다.

## 1. Introduction

The conventional safety or risk analysis is based on deterministic approach, which is too conservative because it considers the uncertainties of the system design or state parameters simultaneously. Nowadays probabilistic and statistical approach is being performed to assess the safety or risk of the nuclear power plant or other engineering system more reasonably.

In the statistical safety assessment, uncertainty analysis plays a very important role. There are three types of uncertainty, namely, modeling uncertainty, parametric uncertainty, and completeness[1]. The modeling uncertainty are analyzed by the change and development of the model. The parametric uncertainty is the one propagated from the uncertainties of the system parameter itself. The completeness is the extent to which the analyzer can recognize the nature of the system. The parametric uncertainty is mainly concerned in this paper.

Various methods to assess the probabilistic risk or uncertainty from the high or low level radioactive waste repository have been proposed [2-6]. Since the system, however, has highly uncertain input parameters, the evaluated risk has high uncertainty. Up to now, there is little work to exploit this problem. Some methods which are used in other fields are adopted and applied to this system in following aspects;

1) to assess the propagated uncertainty from the input parameter uncertainties (uncertainty propagation analysis)

2) to seek for the most dominant factors which contribute the output uncertainty (sensitivity analysis)

3) to construct the reduced system model composed of the most dominant input parameters (model reduction)

For this analysis, statistical package for uncertainty and sensitivity analysis, SPUSA, is developed. SPUSA includes Crude Monte Carlo, Latin Hypercube Sampling, Experimental Design, Analysis of Variance, Response Surface Method, Stepwise Regression Method, and Fourier Amplitude Sensitivity Test, etc.

The probabilistic risk assessment model proposed by Pritzker and Gassmann[2, 3] is used here to discuss the applicability and characteristics of the various uncertainty and sensitivity analysis methods.

## 2. Methods of Uncertainty and Sensitivity Analysis

### 2.1. Three Features of Uncertainty Analysis

Various conventional methods of uncertainty analysis are reviewed in this section. The main features of each method are described at the point of view of the three capabilities mentioned in section 1, i.e., the capabilities of uncertainty propagation analysis, sensitivity analysis, and reduced model construction.

The uncertainty propagation analysis includes the estimation of distribution function of output variable and its representative values, for instance, mean, median, variance, standard deviation, and higher order moments. The Monte Carlo simulation technique is a representative one.

The measure of sensitivity is divided into two categories. One is the differential sensitivity measure, $\frac{dy}{dx_i}\Big|_{x_i=x_i^0}$. Linear sensitivity theory and adjoint sensitivity theory are the representative ones. The other is the global sensitivity measure, $\int \cdots \int \frac{\partial y}{\partial x_i} dx_1 \cdots dx_k$. Fourier Amplitude Sensitivity Test (FAST) is the representative one. The adjoint sensitivity theory[7-9] is a powerful method when the number of input parameters are large, because this method gives the sensitivity of output variable for all the parameters with only single run. A major defect of this method is that each computer program

has to be made for each system model to be analyzed. This method is not considered in this paper, because the purpose of this paper lies on the development of statistical methods.

The methods which have a capability of the reduced model construction are response surface method and stepwise regression technique. These methods also provide sensitivity measure as a byproduct.

Latin hypercube sampling, experimental design technique, and Fourier amplitude sensitivity test are used to generate systematic sampling points. Least square method and analysis of variance are used as a basic tool for response surface method and stepwise regression technique.

### 2.2. Crude Monte Carlo Method[10-12]

Crude Monte Carlo (CMC) method is the most primitive but the most powerful method in uncertainty propagation analysis. First it generates random samples whose size is over than thousands according to the distribution shape of each input parameter. Each random combination of random samples $(x_1^i, x_2^i, \cdots, x_k^i)$, $i=1, \cdots, n$ is passed through the system function to generate corresponding output value $y_i$. The resultant $y_i$'s represents uncertainty distribution of output variable $y$. The mean, variance, and higher order moments of $y$ are calculated from these $y_i$'s. The distribution function of $y$ is obtained directly from these $y_i$'s by making histogram of tens or hundreds of equal intervals. Fig. 2.1 illustrates this process. Sometimes the distribution function of $y$ is matched to an appropriate empirical distribution shape by moment matching technique using some lower order moments calculated above. The major deficiency of CMC method is too much computing cost due to large sample size $n$. Thus it is not used directly in practice. To avoid this problem, the following procedure is usually used. First the complex system function is simplified to an equivalent low order polynomial by response surface technique and then CMC is applied to this polynomial to construct the output distribution.

### 2.3. Latin Hypercube Sampling[13-15]

LHS, which was originally proposed by McKey et al [13], is a kind of variance reduction

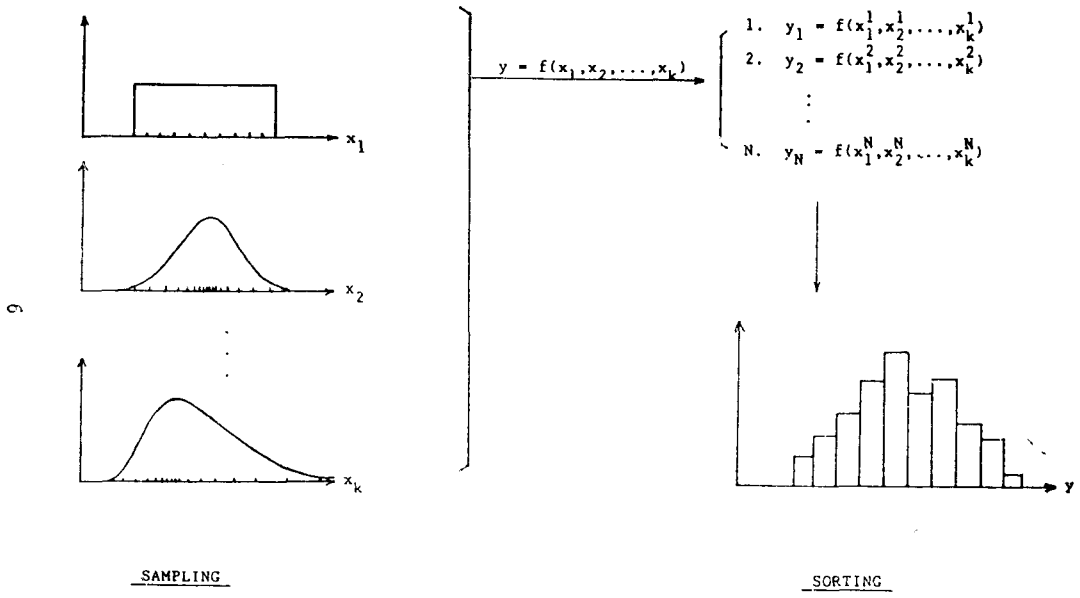


**Fig. 2.1. Crude Monte Carlo Method for Uncertainty Propagation Analysis**

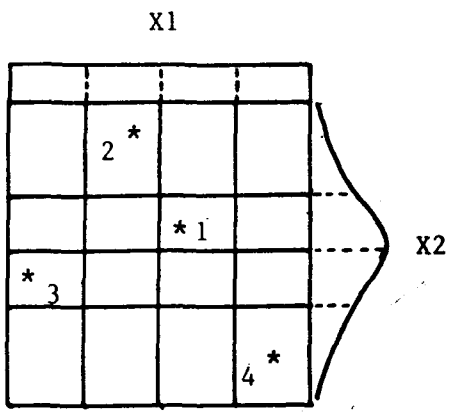


**Fig. 2.2. An Illustration of Latin Hypercube Sampling Points in Two Dimensional Case with n=4.**

technique to generate a sample of size $n$ from $k$ random variables, $X_1, X_2, \cdots X_k$. The range of each variable is divided into $n$ nonoverlapping intervals of equal probability. One value from each interval is selected at random. The $n$ values thus obtained for $X_1$ are paired at random with the $n$ values obtained for $X_2$. These $n$ pairs are combined in a random manner with the $n$ values for $X_3$ to form $n$ triples. The process is continued until a set of $k$-tuples is formed. This resultant set of $k$-tuples is the Latin hypercube sample. Fig. 2.2. illustrates this process in two dimensional case with $n=4$. This technique is good because it samples without undue sampling size $n$. Sample size $n$ is known to be sufficient if $n \geqq 2k$.

**2.4. Experimental Design Techanique**[17~20]

There are several methods in designing experiments to establish a set of sampling points in the space of the $X$'s, at which $Y$ will be observed. The most common of these are two and three level factorial design, two and three level fractional factorial design, and central composite design, which are discussed in this section.

Two level factorial design utilizes two level of $X$'s (coded value of $\pm 1$). When the number of factors (here, number of input parameters) are $k$, the required number of code runs are $2^k$, for the full (complete) factorial design and $2^{k-p}$ for fractional design, where $2^p$ is the fraction needed to reduce the required numbers. In the fractional factorial design, $k-p$ parameters are combined completely but remaining $p$ parameters are composed of product of already defined $k-p$ parameters levels. Obviously, the higher the degree of fraction is, the less is the degree of resolution in analyzing the lower order effects (main or cross term effects compared to the higher order interaction effects).

Three level design is the same as the two level design except that it needs three level of $X$'s $(-1, 0, +1)$. But in these design the number of runs is increasing more rapidly than that of two level design as the number of input parameters increases.

In central composite design, however, three distinct portions are included: (1) two level factorial points, (2) two axial points for each parameters, (3) one center point. Fig. 2-3 illustrates three design points for two factors, where 'a' is an arbitrary coded value.

Among the above mentioned type of experimental designs, the two level factorial design

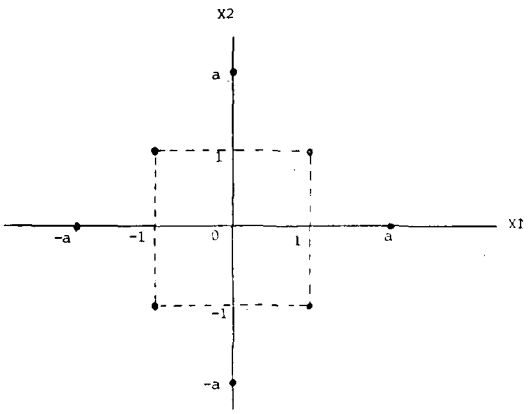


**Fig. 2.3. Central Composite Design Points for Two Factors**

**Table 2-1. Comparison of the Number of Unknowns and Code Runs between Various Experimental Design Techniques**

| No. of Factors $k$ | 1st Order Polynomial | | | 2nd Order Polynomial | | | |
|---|---|---|---|---|---|---|---|
| | No. of Unknown | No. of Runs | | *No. of Unknowns | $3^k$ | No. of Runs | |
| | | $2^k$ | $2^{p-k}$ | | | $3^{k-p}$ | ** |
| 3 | 4 | 8 | $2^{3-1}=4$ | 10 | 27 | — | 15 |
| 4 | 5 | 16 | $2^{4-1}=8$ | 15 | 81 | $3^{4-1}=27$ | 25 |
| 5 | 6 | 32 | $2^{5-1}=16$ | 21 | 243 | $3^{5-1}=81$ | 43 |
| | | | $2^{5-2}=8$ | | | $3^{5-2}=27$ | |
| 7 | 8 | 128 | $2^{7-1}=64$ | 36 | 2187 | $3^{7-1}=729$ | 143 |
| | | | $2^{7-2}=32$ | | | $3^{7-2}=243$ | |
| | | | $2^{7-3}=16$ | | | $3^{7-3}=81$ | |
| | | | $2^{7-4}=8$ | | | | |

* $2k+{}_kC_2+1$

** (Central Composite Design) $2^k+2k+1$

and the central composite design are most commonly used for response surface work. The reason is that the former can be used to fit first order polynomial with minimum number of code runs, while the latter is suitable for fitting the second order polynomial. The major advantage of the central composite design is utilizing the information of two level design to consider the nonlinearity with a few additional data points in case that the constructed linear model is not satisfying.

Table 2-1 shows the comparison of the number of unknowns and code runs required for these experimental design methods. It is obvious that the central composite design needs relatively few number of runs compared to the three level factorial design.

### 2.5. Response Surface Method [16~18]

This method is usually used to generate an approximate relationship between the input parameters and the output variable considering the system as a blackbox.

When the output variable $y$ is a complex function of a number of input parameters, $x_i$ $(i=1, 2, \cdots, k)$, say,

$$y=f(x_1, x_2, \cdots, x_k), \quad (2.1)$$

the input-output relationship can be approximated in the form of polynomial as

$$y=b_0+\sum_i^k b_i x_i, \quad \text{(1st order regression)} \quad (2.2)$$

or

$$y=b_0+\sum_i^k b_i x_i+\sum_{i<j}\sum^k b_{ij} x_i x_j, \quad \text{(2nd order regression)} \quad (2.3)$$

where

$$x_i=\frac{z_i-z_i^0}{\Delta z_i}=\text{coded value or level}, \quad (2.4)$$

$z_i$=real value,

$z_i^0$=nominal value,

$\Delta z_i$=unit deviation.

The term response surface refers to the geometrical interpretation of a function of several independent variables. If the functional relationship is not highly nonlinear in the interested region of independent variables, then the first order regression equation can be used. Otherwise, the second or higher order regression equation will fit the relationship reasonably. Sometimes even in case that the nonlinearity is obvious in the wide range of independent variables, the first order model can be used in the narrow interested region of independent variables.

It is the purpose of RSM to generate a simplified polynomial equation from sampled data set and to extract information for the unknown

system from this response surface equation. The coefficients are obtained by the least square method and the characteristic features of the system are extracted by using analysis of variance (ANOVA). ANOVA is described in the following section. To generate a sample without computer simulation, EDT described in the previous section is usually used.

### 2.6. Multiple Least Square and Analysis of Variance [17, 21, 22]

Eqs. (2.2) and (2.3) can be represented by matrix form as

$$y=Xb+e, \tag{2.5}$$

where

$y=n\times 1$ observed data vector,

$X=n\times m$ design matrix,

$b=m\times 1$ coefficient vector,

$e=n\times 1$ error vector, i.e. the difference between observed data and estimated response,

$n=$number of observations (runs),

$$m=\begin{cases} 1+k, & \text{for 1st order regression,} \\ 1+2k+{}_kC_2, & \text{for 2nd order regression.} \end{cases}$$

The best-estimated regression coefficients $b$ can be found by the method of least squares. If sum of squares of the error

$$L=e^Te=(y-Xb)^T(y-Xb) \tag{2.6}$$

is minimized, i.e., $\frac{\partial L}{\partial b}=0$, then the regression coefficient is represented by

$$b=(X^TX)^{-1}X^Ty. \tag{2.7}$$

The analysis of variance (ANOVA) is to distinguish between the variation due to regression and the variation due to residual errors from the total variation. Fig. 2.4 illustrates this for the single variable case.

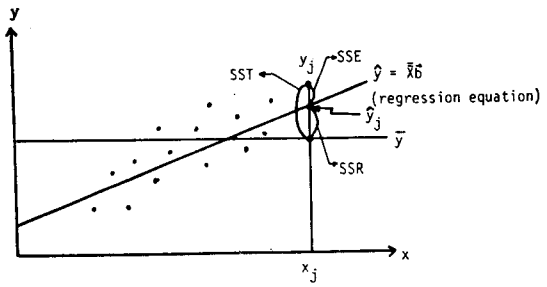


**Fig. 2.4. An Illustration of Analysis of Variance For Single Factor Case**

Total variation is usually called total sums of squares (SST) and is defined by

$$\begin{aligned} SST&=\Sigma(y_j-\bar{y})^2=\Sigma y_j^2-n(\bar{y})^2 \\ &=y^Ty-n(\bar{y})^2. \end{aligned} \tag{2.8}$$

Variation due to regression equation is called sum of square due to regression (SSR) and is defined by

$$\begin{aligned} SSR&=\Sigma(\hat{y}_j-\bar{y})^2=\Sigma\hat{y}_j^2-n(\bar{y})^2 \\ &=\hat{y}^T\hat{y}-n(\bar{y})^2. \end{aligned} \tag{2.9a}$$

Since $y=Xb$,

$$SSR=b^TX^Ty-n(\bar{y})^2. \tag{2.9b}$$

Finally, sum of squares due to residual errors (SSE) can be represented by

$$SSE=SST-SSR. \tag{2.10}$$

The degree of freedoms for total variation, regression equation, and residual errors are $n-1$,

**Table 2-2. ANOVA Table for Multiple Regression**

| Source | S.S | D.F | M.S | F | Critical-F | $R^2$ |
|---|---|---|---|---|---|---|
| Regress. | SSR | $k$ | MSR | (MSR/MSE) | $F(k, n-k-1;\alpha)$ | (SSR/SST) |
| Error | SSE | $n-k-1$ | MSE | | | |
| Total | SST | $n-1$ | | | | |

where S.S =Sum of Squares
D.F=Degree of Freedom
M.S=Mean of Squares=(S.S/D.F)
$n$=number of observations (runs)
$k$=number of regression factors
$R^2$=coefficient of determination

$k$, and $n-k-1$, respectively. From these information, ANOVA table for multiple regression can be made as shown in Table 2.2.

There are three measures which describes the accuracy of regression equation to the observed data. These are MSE (mean of squares due to residual error), $F$(=MSR/MSE), and $R^2$(= SSR/SST, so called, coefficient of determination). The smaller MSE is, the better is regression, while the reversed situation is applied for $F$ and $R^2$. It is called that the regression is significant at a level of $100(1-\alpha)$ % if

$$F>F(k, n-k-1\ ;\ \alpha), \tag{2.11}$$

When the significance of each component (main effect term, quadratic term, cross-term) of regression is considered, partial $F$-test can be applied, which is defined by

$$F_i=\frac{b_i^2}{(X^TX)_{ii}^{-1}(\mathrm{MSE})}. \tag{2.12}$$

It is also called that the component $x_i$ is significant at a level of $100(1-\alpha)$ % if

$$F_i>F(1, n-k-1\ ;\ \alpha). \tag{2.13}$$

**2.7. Stepwise Regression Technique**[17, 21, 22]

SRT is used to select the most important input parameters, thereby to build regression equation composed of not an undue number of input parameters while the constructed regression equation reveals the input-output relationship. This procedure selects or removes the most important or the least important input parameter sequentially. At each step to decide the adequacy of the construeted regression model composed of the selected input parameters, ANOVA is used.

In selecting an input parameters at each step, partial $F$ value is used. The input parameter which has the largest partial $F$ value is selected. For the selected input parameter, $F$ test is performed. If $F_i>F(1, n-p-1\ ;\ \alpha)$, where $p$ is the number of input parameters included in the regression model, the input parameter is included in the model and then go to next step. Otherwise, the procedure is stopped here. The meaning is that the input parameter inclusion is significant at a level of $100\alpha$ %.

**2.8. Fourier Amplitude Sensitivity Test** [23-28]

Consider a system that is described by an ordinary differential equations containing $k$ input parameters, $x_1, x_2, \cdots, x_k$,

$$\frac{dy}{dt}=f(y\ ;\ x_1, \cdots, x_k), \tag{2.14}$$

where

$y$=interested system output at time $t$,

$\vec{x}$=$k$-dimensional parameter vector.

The basic problem is to determine the sensitivity of $y$ to simultaneous variations in all the parameters $\vec{x}$. This is done by considering that $\vec{x}$ has a distribution of values resulting from either imprecision or uncertainty in their definition. The ensemble mean value of $y$ is then given by

$$\langle y\rangle=\int\cdots\int y(t\ ;\ x_1, \cdots x_k)\ p(x_1, \cdots, x_k)\ dx_1\cdots dx_k, \tag{2.15}$$

where

$y(t\ ;\ x_1, \cdots, x_k)$=the solution of Eq. (2.14),

$p(x_1, \cdots, x_k)$=joint probability density function of $\vec{x}$.

The central idea of the FAST method is to convert the $k$-dimensional integral of Eq. (2.15) into an equivalent one-dimensional form by using the transformation

$$x_i=G_i[\sin(w_i s)],\quad i=1, \cdots, k \tag{2.16}$$

where

$G_i$=a set of known functions,

$w_i$=a set of frequencies,

$s$ =a scalar variable.

By means of this transformation, the variations of the $k$ parameters are transformed into variations of the single scalar variable $s$. By variation of $s$ over the range $-\infty\leq s\leq\infty$, Eq. (2.16) traces out a space-filling curve in the $m$-dimensional parameter space. For a suitable choice of $G_i$, which transforms the probability density function $p(\vec{x})$ into $s$-space, Weyl demonstrated that

$$\bar{y}=\lim_{T\to\infty}\frac{1}{2T}\int_{-T}^{T}y(t\,;\,x_1(s),\cdots,x_k(s))ds \tag{2.17}$$

is identically equal to $\langle y\rangle$ in Eq. (2.15). Eq. (2.17) is the fundamental expression in the FAST method for computing the mean value, variance, and other properties of the output $y$.

By using an appropriate integer frequency set $\{w_i\}$, the parameters, $x_i$ are periodic in $s$ on the finite interval $(-\pi,\pi)$, in which case Eq. (2.17) becomes

$$\bar{y}=\frac{1}{2\pi}\int_{-\pi}^{\pi}y(t\,;\,x_1(s),\cdots,x_k(s))ds. \tag{2.18}$$

The variance of $y$ is then

$$\sigma_y^2=\frac{1}{2\pi}\int_{-\pi}^{\pi}y^2(t\,;\,x_1(s),\cdots,x_k(s))ds-(\bar{y})^2$$
$$=\bar{y}^2-(\bar{y})^2. \tag{2.19}$$

The evaluation of $\sigma_2{}^y$ can be carried out by using the $s$-space Fourier coefficients of $y$. From Parseval's theorem,

$$\bar{y}_2=\frac{1}{2\pi}\int_{-\pi}^{\pi}y^2\,ds=\sum_{j=-\infty}^{\infty}(A_j^2+B_j^2) \tag{2.20}$$

where the Fourier coefficients $A_j$ and $B_j$ are defined by

$$A_j=\frac{1}{2\pi}\int_{-\pi}^{\pi}y\cos(js)\,ds, \tag{2.21}$$

$$B_j=\frac{1}{2\pi}\int_{-\pi}^{\pi}y\sin(js)ds. \tag{2.22}$$

Thus, from Eq. (2.21) and (2.22)

$$(\bar{y})^2=A_0^2+B_0^2=A_0^2. \tag{2.23}$$

Then,

$$\sigma_y^2=2\sum_{j=1}^{\infty}(A_j^2+B_j^2). \tag{2.24}$$

The variances due to $w_i$ and its harmonics are expressed by

$$\sigma_{wi}^2=2\sum_{k=1}^{\infty}(A_{kwi}^2+B_{kwi}^2). \tag{2.25}$$

The normalized sensitivity measure, partial variance, $S_{wi}$, is defined by the ratio of the variance due to the frequency $w_i$ to the total variance as follows:

$$S_{wi}=\frac{\sigma_{wi}{}^2}{\sigma_y{}^2}. \tag{2.26}$$

Restricting the frequency set to odd integers reduces the range of $s$ to $[-\pi/2,\ \pi/2]$. In this case,

$$y(\pi-s)=y(s),$$
$$y(\pi+s)=y(-s),$$
$$y(\pi/2+s)=y(\pi/2-s),$$
$$y(-\pi/2+s)=y(-\pi/2-s), \tag{2.27}$$

and the Fourier coefficients can be expressed as

$$A_j=\begin{cases}0 & ;\ j\ \text{odd}\\ \frac{1}{\pi}\int_0^{\pi/2}[y(s)-y(-s)]\cos(js)ds & ;\ j\ \text{even},\end{cases} \tag{2.28}$$

$$B_j=\begin{cases}0 & ;\ j\ \text{even}\\ \frac{1}{\pi}\int_0^{\pi/2}[y(s)-y(-s)]\sin(js)ds & ;\ j\ \text{odd}.\end{cases} \tag{2.29}$$

This can be further reduced by a simple numerical quadrature as

$$A_j=\begin{cases}0 & ;\ j\ \text{odd}\\ \frac{1}{2n+1}\left\{y_0+\sum_{k=1}^{n}(y_m+y_{-m})\cos\left(\frac{jm\pi}{2n+1}\right)\right\} & ;\ j\ \text{even},\end{cases} \tag{2.30}$$

$$B_j=\begin{cases}0 & ;\ j\ \text{even}\\ \frac{1}{2n+1}\left\{\sum_{k=1}^{n}(y_m-y_{-m})\sin\left(\frac{jm\pi}{2n+1}\right)\right\} & ;\ j\ \text{odd},\end{cases} \tag{2.31}$$

where $y_m(-n\le m\le n\,;\,n=\omega_{\max})$ is the $y$ which is calculated at an input set $x_i^m=G_i\left\{\sin\left(\omega_i\frac{m\pi}{2n+1}\right)\right\}$, $i=1,2,\cdots,k$.

It is sufficient if the total sampling points are determined by $N_s=2\omega_{\max}+1$ by the Nyquist criterion in the digital signal processing theory.

The rapidly-decaying properties of the Fourier Amplitudes provide that the summation to $k=2$ is sufficient in calculation of $\sigma_{wi}{}^2$ of Eq. (2.25), that is,

**Table 2.3. Integer Frequency Sets and Number of Sampling Points**

| Number of Variables | Integer Frequenc Set $\{\omega_i\}$ | Minimum Sampling Points |
|---|---|---|
| 5 | 11, 21, 27, 35, 39 | 79 |
| 6 | 1, 21, 31, 37, 45, 49 | 99 |
| 7 | 17, 39, 59, 69, 75, 83, 87 | 175 |
| 8 | 23, 55, 77, 97, 107, 113, 121, 125 | 251 |
| 9 | 19, 59, 91, 113, 133, 143, 149, 157, 161 | 323 |
| 10 | 25, 63, 103, 135, 157, 177, 187, 193, 201, 205 | 411 |
| 11 | 41, 67, 105, 145, 177, 199, 219, 229, 235, 243, 247 | 495 |
| 12 | 31, 87, 113, 151, 191, 223, 245, 265, 275, 281, 289, 293 | 587 |
| 13 | 23, 85, 141, 167, 205, 245, 277, 299, 319, 329, 335, 343, 347 | 695 |
| 14 | 87, 133, 195, 251, 277, 315, 355, 387, 409, 429, 439, 445, 453, 457 | 915 |
| 15 | 67, 143, 189, 251, 307, 333, 371, 411, 443, 465, 485, 495, 501, 509, 513 | 1,027 |
| 16 | 73, 169, 245, 291, 353, 409, 435, 473, 513, 545, 567, 587, 597, 603, 611, 615 | 1,231 |
| 17 | 85, 145, 241, 317, 363, 425, 481, 507, 545, 585, 617, 639, 659, 669, 675, 683, 687 | 1,375 |
| 18 | 143, 229, 289, 385, 461, 507, 569, 625, 651, 686, 729, 761, 783, 803, 813, 819, 827, 831 | 1,663 |
| 19 | 149, 275, 361, 421, 517, 593, 639, 701, 757, 783, 821, 861, 893, 915, 935, 945, 951, 959, 963 | 1,927 |

$$\sigma_2^{wi}=2(A_2^{1wi}+B_2^{2wi}). \quad (2.32)$$

The interference problem, which is caused by multiples of harmonics between different integer frequencies, can be avoided up to a certain degree (order) if the integer frequency sets are selected as follows:

$$i\cdot\omega_1+j\cdot\omega_m\neq k\cdot\omega_n, \quad i,j,k=0,1,2,3,4,\cdots. \quad (2.33)$$

The integer frequency sets which avoid the interference problem up to 4th order are shown in Table 2.3.

## 3. Uncertainty Analysis for High Level Waste Repository

### 3.1. Introduction

Various methods to assess the probabilistic risk or uncertainty from the high or low level radioactive waste repository have been proposed [29~31]. Since the system has highly uncertain input parameters, the evaluated risk has also high uncertainty. Up to now, there is little work to exploit this problem. Since both the input parameters and the output variable of this system have highly nonlinear natures, the conventional techniques cannot be used directly any more. Therefore, some different techniques are developed in this paper to be applicable to highly nonlinear system models. The probabilistic risk assessment model proposed by Pritzker and Gassmann [2, 3] is used here.

### 3.2. Assumed Radioactive Waste Repository System and Scenario of Radioactivity Release

Radioactive waste repository must be located in a geological formation which is quite stable tectonically, and at which the probabilities of the occurrence of an earthquake and a fault are very low. The waste disposal stratum is located about 600m below the ground surface and the type of stratum generally chosen is rock salt to prevent the intrusion of the ground water.

The waste repository is composed of parallel disposal tunnels for the emplacement of waste

and shafts for the linkage to the ground surface. On the ground of the disposal tunnel, many vertical holes are drilled for the disposal of high level waste canisters. The space between the wall of the hole and the canister is packed with backfill materials such as bentonite, zeolite, etc. After the canisters are put in all the holes in the tunnels, the disposal tunnels are packed with buffer material such as a mixture of quartz sand and bentonite, etc. When the entire repository is filled, the shaft and other spaces are also packed with the same buffer materials.

The underground radioactive waste repository consists of five barriers to isolate the high-level radioactive waste from the biosphere.

1) barrier A: host rock (rock salt or crystalline rock, etc.)
2) barrier B: waste canister (Ti-Pb container)
3) barrier C: waste glass (borosilicate glass)
4) barrier D: backfill (bentonite)
5) barrier E: geological structure between repository and biosphere (granite)

At the beginning of the release, host rock (barrier A) where the waste repository is located, is failed by artificial or natural events (drilling, earthquake, brine migration, etc.) and some groundwater in the geological stratum surrounding the host rock intrudes into the waste repository. The space between the host rock and the wall of the waste canister is filled with backfill materials such as bentonite. After the saturation of backfill with groundwater, groundwater contacts with and corrodes the waste canister (barrier B). As corrosion proceeds, ground water will eventually come into contact with the waste glass (barrier C). High level waste glass is a homogeneous glass so-called "borosilicate." In case of long contact with groundwater, the waste glass is leached out at a very slow rate. The nuclides leached from the waste glass are retarded for a considerable period by adsorption as they pass through the backfill (barrier D). After passing through backfill, this groundwater reaches the ground surface or surface water through geological structure (barrier E), while the radioactive nuclides along the same path but are retarded by adsorption.

### 3.3. Reliability and Risk Assessment Model

In the system in continuous operation without repair, the failure probability density $f(t)$ is [32]

$$f(t)=\lambda(t)\exp[-\int_0^t\lambda(t')dt'] \tag{3.1}$$

and the mean-time-to-failure (MTTF) is

$$\text{MTTF}=\int_0^\infty tf(t)dt, \tag{3.2}$$

where

$\lambda(t)$=hazard rate or conditional failure rate.

If the failure of the system occurs randomly, then

$$\lambda(t)=\lambda, \tag{3.3}$$

$$f(t)=\lambda\ \exp(-\lambda t), \tag{3.4}$$

$$\text{MTTF}=1/\lambda. \tag{3.5}$$

For the system in which components are sequential in operation in such a way that the only one unit of the system is in operation at a time [32],

$$f_{sys}(t)=\int_0^t f_1(t_1)\int_{t_1}^t f_2(t_2-t_1)\cdots\cdots \int_{t_{N-2}}^t f_{N-1}(t_{N-1}-t_{N-2})f_N(t-t_{N-1})\,dt_{N-1}dt_{N-2}\cdots dt_1 \tag{3.6}$$

If the hazard rate is assumed constant in time, then

$$f_{sys}(t)=[\prod_{i=1}^N\lambda_i]\sum_{i=1}^N\frac{e^{-\lambda_i t}}{\prod_{j\neq i}^N(\lambda_j-\lambda_i)}. \tag{3.7}$$

The risk from the radioactivity release from the waste repository can be represented by

$$R_k(t)=A_k(t)f_{sys}(t)=A_k(0)\ \exp(-\lambda_k t)f_{sys}(t), \tag{3.8}$$

where

$R_k(t)$ =probable release rate of radioactive nuclide $k$ at time $t$ $(Ci/yr)$,

$A_k(0)=\lambda_K N_K(0)$=initial activity of the nuclide $k$ $(Ci)$,

$N_k(0)$ =inventory of the nuclide $k$ at time $t=0$, when the waste is disposed of in the disposal site,

$\lambda_k$ =decay constant of the nuclide $k$ $(1/yr)$.

### 3.4. Failure Probability of Each Barrier

As described in the previous sections, only risks due to transportation and release of radioactive nuclides to biosphere by the groundwater are considered. The waste repository is considered as a system in continuous operation, whereby five units are in a sequential operation mode. At first, we consider the reliabilities of the single barrier. In the second step, we consider the overall reliabilities of the waste repository using the reliability of the single barrier.

Barrier A (Host Rock)

The failure of barrier A means the intrusion of the groundwater that exists in the aquifer above or below the host rocks, to the backfill between host rock and waste canister through the host rock. This failure is due to many different causes, for example, undetected borehole, fracture, etc. Such phenomena will be likely to occur randomly. The overall MTTF is to be determined based on experience and geological knowledge. In many studies, it was assumed for groundwater in the aquifer to intrude into the waste repository after a period varying between 10 and 1,000 yrs [33, 36].

Barrier *B* (Waste Canister)

After barrier *A* is failed, the groundwater contacts with the waste canister. The failure of the waste canister is mainly due to the corrosion of the canister material by the groundwater. The waste canisters are largely titanium-lead containers. Many corrosion studies showed that the life time of titanium alloys is 300~3,000 years. [34, 39]

Barrier *C* (Waste Glass)

Failure of barrier *C* means leaching of radioactive material in waste glass. The leaching process is dominated by the dissolution of waste glass and it is a function of the amount in contact with groundwater, the leaching rate, and the surface-to-volume ratio of the solid [37]. Then, the MTTF of barrier *C* in cylindrical form can be represented as follows [2, 3].

$$\begin{aligned}\mathrm{MTTF}_c &= \frac{1}{m_0}\int_0^{t_m} t\left(\frac{dm}{dt}\right)dt \\ &= \frac{1}{m_0}\int_0^{t_m} t\cdot 2\left(\frac{m_0}{t_m}\right)\left(1-\frac{t}{t_m}\right)dt \\ &= \frac{t_m}{3}, \end{aligned} \tag{3.9}$$

where

$m_0$=initial mass of waste glass,

$t_m$ =total dissolution time of waste glass.

It is reported that the total dissolution time of borosilicate glass is about 10,000~100,000 years [39].

Barrier *D* (Backfill)

Backfill acts as a barrier in two manners: namely, to prevent groundwater intrusion into the waste canister when the failure of barrier *A* occurs, and to retard radionuclide migration when the leaching of the waste glass occurs.

In the former case, for a backfill thickness of 0.25m, if the waste repository is located at the depth of 1,000m underground, the maximum time for water to saturate the backfill will be about 20 years [35]. This is much shorter than the time scale used in the other barriers. Accordingly this function is neglected here.

In the latter case, it is reported that a porous backfill should have low permeability enough to prevent transport of radionuclides by the bulk fluid flow, and the transport of water will be controlled by diffusion through the pore, provided that the physical integrity of the backfill is maintained [35, 38]. In the case of diffusion of radionuclides through the backfill, modified Fick's second law is applied with the assumption of infinite diffusion medium [35].

$$\frac{\partial C}{\partial t} = \left(\frac{D}{K_R\tau}\right)\frac{\partial^2 C}{\partial X^2}, \tag{3.10}$$

where

$D$ =diffusivity=$10^{-9}$m$^2$/sec,

$\tau$ =tortuosity factor=1,

$X$ =distance (=0.25m, thickness of backfill),

$K_R$=retardation factor of each nuclide,

$C$ =nuclide concentration.

With following bouudary conditions and initial condition,

$$C(0,t)=C_0,\quad C(\infty,t)=0,\quad C(x,0)=0$$

the solution to Eq. (3.10) is then

$$C=C_0 \text{ er } fc\left[\frac{X}{2\left(\frac{Dt}{K_R\tau}\right)^{\frac{1}{2}}}\right]. \qquad (3\cdot11)$$

Therefore, the diffusion time of radionuclide, $t_d$, which is defined as the time that radionuclides pass through the backfill, is mainly a function of retardation factor. The MTTF of barrier $D$ can be represented by [2].

$$\text{MTTF}_D=t_d/2\cong K_R/8. \qquad (3.12)$$

Barrier $E$ (Geological Structure)

The radioactive nuclides released from the waste repository are transported through geological structure by means of groundwater and released to the biosphere. Many studies [33, 40, 41] assume that ground water reaches a river or a lake after 200~2000 years while the radioactive material migrates along the same path but is retarded by adsorption process. Also it is assumed that radioactive nuclides are only retarded but undiminished by chemical process. The failure mechanism of the barrier $E$ can be assumed random failure and MTTF is represented by the mean migration time of nuclides as follows [2, 3]

$$\text{MTTF}_E=K_R T_W, \qquad (3.13)$$

where

$T_W$=travel time of groundwater=200~2,000 years,

$K_R$=retardation factor for each nuclide.

### 3.5. Radionuclide Inventory in Waste Repository

The radionuclide inventories in high level waste disposed in the waste repository are varied with the time duration after burial. These inventories can be calculated as a function of time after the removal of fuel from the reactor. These calculations were carried out by the use of ORIGEN code [42]. The reactor parameters used in these calculations are as follows: uranium enrichment of a fuel, 3.2% U-235, average power 30MW/MT, exposed time 1,100 days. It is assumed that spent fuel is reprocessed 160 days after removal from the reactor. The probable release rate of the radionuclides are calculated based on 10 PWRs with 1,000MW and 40 years of operation. Assuming 30 tons of spent fuel per reactor year, the inventory amounts to 12,000 ton Uranium. This corresponds to a repository with roughly 5,000 waste canisters.

### 3.6. Results and Discussions

In the assessment of the risk from the high level radioactive repository, the MTTF of each barrier is decided to be fundamental parameters which have uncertainties. The uncertainty ranges of input parameters obtained from various reports are shown in Table 3.1 and 3.2. The important nuclides for ingestion are considered in this study and they are listed in Table 3.2 with their half lives, initial inventories, and ratardation factors. In the calculation, all the parameters are assumed to have 'loguniform' distributions because the ranges spread in order-of-magnitudes. The assumption of loguniform distribution gives more conservative results than that lognormal distribution which is usually used in reliability assessments of nuclear power plants. The transformation of original independent variable $X_i$ logarithmically based on 10 results in uniform distribution.

$$X_i'=\log(X_i)\sim U, \qquad (3.14)$$

$$Z_i=\frac{X_i'-\overline{X_i'}}{\Delta X_i'}\sim U(-1,1), \qquad (3.15)$$

where

$X_i'$=logarithmically transformed variable of $X_i$,

$Z_i$ =normalized variable of $X_i'$,

$U(a, b)$=uniform distribution between $a$ and $b$.

The output variable $Y$ is also transformed logarithmically because it is expected that $Y$ also spreads in order-of-magnitudes. Use of logarithmic transformation reduces nonlinear effect and thus the result can be interpreted in linear base.

**Table 3.1. Uncertainty Range of Input Parameters**

| Parameter | Uncertainty Range |
|---|---|
| $X_1$ ($MTTF_A$) | 1E+1~ 1E+3 yr |
| $X_2$ ($MTTF_B$) | 3E+2~ 3E+3 yr |
| $X_3$ ($MTTF_C$) | 3.3E+3~3.3E+4 yr |
| $X_4$, $X_5$ | in Table 3.2 |

**Table 3.2. Initial Activity, Half Life, and Retardation Factors for Barrier *D* and *E* of Each Nuclide**

| Nuclide | Initial Activity (Ci) | Half Life (yr) | $X_4$=KR (Barrier *D*) ($MTTF_D$ =KR/8) | KR (Barrier *E*) | $X_5$=TW. KR ($MTTF_E$) (yr) |
|---|---|---|---|---|---|
| Sr-90 | 3.387E+4 | 29 | 1E+3~2E+3 | 2E+1~1E+2 | 4E+3~2E+5 |
| Tc-99 | 5.376E+4 | 2.13E+5 | 1E+0~1E+2 | 1E+0~1E+1 | 2E+2~2E+4 |
| Cs-137 | 4.010E+4 | 30.14 | 1E+2~1E+4 | 1E+2~1E+3 | 2E+4~2E+6 |
| Ra-226 | 3.960E−3 | 4.50E+9 | 1E+3~2E+3 | 3E+2~1E+3 | 6E+4~2E+6 |
| Np-237 | 1.320E+3 | 2.10E+6 | 2E+2~8E+2 | 1E+2~3E+2 | 2E+4~6E+5 |
| Pu-240 | 3.116E+4 | 6,500 | 2E+3~5E+3 | 3E+2~1E+3 | 6E+4~2E+6 |
| Am-241 | 6.000E+5 | 430 | 1E+4~2E+4 | 1E+3~1E+5 | 2E+5~2E+8 |

The FAST results for Sr-90 are shown in Fig. 3-1 with the mean and the most extreme output values. The results are in good agreement

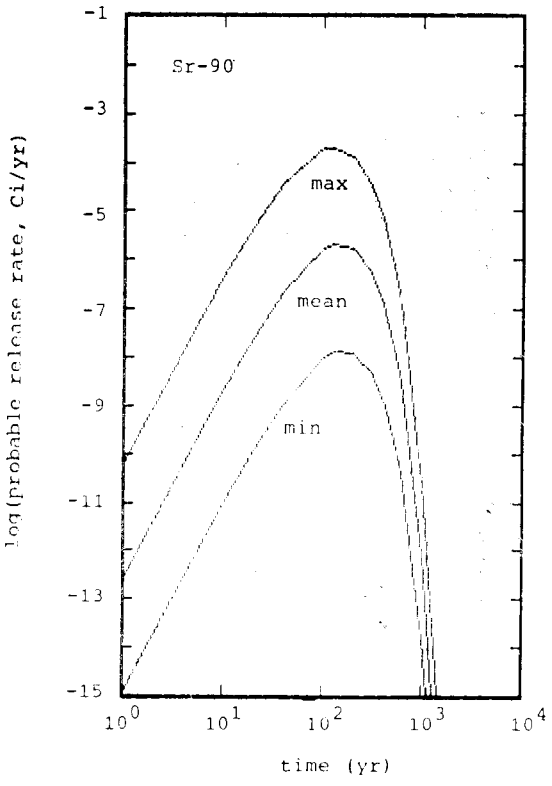


**Fig. 3.1. Probable Release Rate of Sr-90 Estimated by FAST**

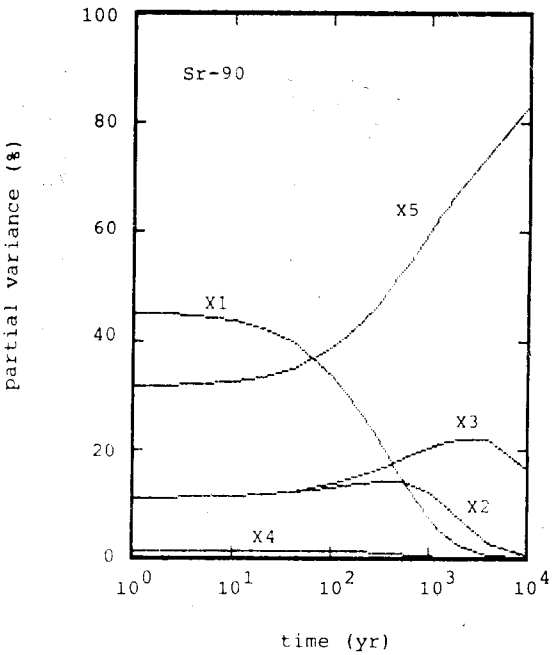


**Fig. 3.2. Partial Variance of Each Input Parameter for Sr-90 Estimated by FAST**

with those estimated by the Monte cario Method of sampling size 2000, which is not shown in the figure. The required number of function evaluations in FAST is 79 for five parameter case as shown in Table 2-3. The resulss for the other nuclides are shown in Appendix. The probable release rates of each nuclide are distributed in three to six order-of-magnitudes during generating period (the time duration in which release rates are increasing) depending on the uncertainty ranges of input parameters. For long lived nuclides, such as Tc-99, Np-237, and Ra-226, however, the probable release rates are rather widely distributed during decaying period after about $10^4$ years. This is mainly due to the long MTTF of barrier E. The results reveal that log $(Y)$ to be nearly normally distributed during generating period. This gives the justification that logarithmic transformation can be used in case that the variables are distributed in order-of-magnitudes. And the resulting normal distribution can be expected from Central Limit Theorem [43]. The time dependent partial variances for input parameters estimated by FAST are shown in Fig. 3-2. This figure explains the uncertainty contributions of each parameter. The

**Table 3-3. Normalized Latin Hypercube Sampling Points and Output Values for Sr-90 at 10yr**

| Run No. | Z1 | Z2 | Z3 | Z4 | Z5 | Y |
|---|---|---|---|---|---|---|
| 1 | 0.414 | −0.894 | −0.633 | −0.880 | −0.824 | −7.480 |
| 2 | 0.475 | 0.016 | −0.062 | −0.766 | −0.206 | −8.821 |
| 3 | −0.870 | −0.640 | 0.819 | 0.347 | 0.250 | −8.200 |
| 4 | 0.918 | 0.883 | 0.159 | 0.060 | −0.282 | −9.863 |
| 5 | −0.513 | 0.173 | 0.240 | −0.142 | −0.100 | −8.270 |
| 6 | 0.396 | 0.230 | 0.064 | 0.246 | −0.458 | −8.847 |
| 7 | 0.703 | −0.700 | −0.343 | −0.234 | −0.641 | −8.259 |
| 8 | 0.655 | −0.386 | 0.949 | −0.958 | −0.909 | −8.678 |
| 9 | −0.582 | −0.741 | 0.095 | 0.190 | 0.522 | −8.255 |
| 10 | −0.814 | −0.158 | −0.132 | 0.591 | −0.149 | −7.711 |
| 11 | −0.161 | −0.104 | −0.756 | 0.124 | 0.288 | −8.339 |
| 12 | −0.325 | −0.806 | −0.459 | −0.080 | 0.387 | −8.033 |
| 13 | −0.666 | 0.543 | 0.897 | −0.417 | 0.195 | −8.850 |
| 14 | −0.703 | −0.542 | 0.608 | −0.313 | −0.549 | −7.515 |
| 15 | −0.374 | −0.471 | −0.927 | 0.300 | 0.653 | −8.201 |
| 16 | 0.041 | 0.824 | 0.572 | −0.362 | −0.395 | −9.011 |
| 17 | 0.199 | 0.300 | 0.327 | 0.902 | 0.889 | −10.062 |
| 18 | 0.821 | 0.414 | 0.773 | −0.553 | 0.697 | −10.580 |
| 19 | −0.421 | 0.118 | −0.286 | −0.499 | −0.032 | −8.071 |
| 20 | 0.996 | −0.981 | −0.846 | 0.608 | −0.674 | −8.258 |
| 21 | −0.048 | 0.795 | 0.527 | 0.787 | 0.858 | −10.122 |
| 22 | 0.735 | −0.036 | 0.438 | 0.972 | −0.951 | −8.929 |
| 23 | −0.961 | 0.522 | 0.338 | −0.691 | 0.131 | −8.206 |
| 24 | −0.211 | 0.656 | −0.588 | −0.064 | 0.557 | −8.954 |
| 25 | −0.127 | 0.952 | −0.218 | 0.681 | 0.064 | −9.061 |
| 26 | −0.780 | −0.274 | −0.975 | 0.412 | −0.475 | −6.959 |
| 27 | 0.265 | 0.395 | −0.157 | 0.486 | −0.766 | −8.464 |
| 28 | 0.591 | −0.427 | −0.690 | −0.617 | 0.953 | −9.407 |
| 29 | 0.313 | −0.236 | −0.508 | −0.858 | 0.769 | −9.126 |
| 30 | 0.072 | 0.712 | 0.719 | 0.864 | 0.461 | −9.969 |

**Table 3-4. Results of Stepwise Regression Analysis for Sr-90 at 10yr**

| Step | Selected Variables | Regression Coefficients | $R^2$ | Partial F | Critical F |
|---|---|---|---|---|---|
| 1st | | −8.675 | | | |
| | Z2 | −0.890 | 0.375 | 16.8 | 2.89 |
| 2nd | | −8.675 | | | |
| | Z2 | −0.896 | | | |
| | Z1 | −0.734 | 0.635 | 19.2 | 2.90 |
| 3rd | | −8.675 | | | |
| | Z2 | −0.736 | | | |
| | Z1 | −0.913 | | | |
| | Z5 | −0.776 | 0.895 | 64.6 | 2.91 |
| 4th | | −8.675 | | | |
| | Z2 | −0.529 | | | |
| | Z1 | −0.956 | | | |
| | Z5 | −0.844 | | | |
| | Z3 | −0.489 | 0.990 | 238. | 2.92 |

MTTF of barrier A (Z1) prevails initially while MTTF of barrier E (Z5) later.

Next, Latin hypercube sampling and stepwise regression is performed sequentially. The normalized Latin hypercube sampling points ($Z_i$) are shown in Table 3-3 with their resulting output value, the probable release rate of Sr-90 at time 10yr. The sequential results of stepwise regression analysis are shown in Table 3-4. Z2, Z1, Z5, and Z3 are sequentially selected at each step. This is a little different from the results estimated by FAST as shown in Fig. 3-2. However, the orders of standardized regression coefficients ($B_i$) become the same as the partial variances of FAST as step goes on. The major merit of FAST method is that it can estimate the sensitivities of each input parameter in the sense of variance, whereas it can not be detected by the Monte Carlo Method.

It can be concluded that FAST is a good method because it gives partial variance of each input parameter, which can be considered as global sensitivity measure, as well as total variance with moderate computing cost compared to Crude Monte Carlo method. Latin hypercube sampling plus stepwise regression procedure gives an alternative tool for uncertainty and sensitivity analysis. Although the test results are not shown in this paper, it is turned out that the Experimental Design plus Response Surface Method is good in case that there is no high nonlinearity in the interested region of input parameter space [44]. Among the methods introduced in section 2, any other combination is possible. The use of any combination can be changed from case to case depending on the nature of the system to be analyzed.

The SPUSA package is expected to be a useful tool for structural analysis of a newly developed uncertain system models.

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## Appendix

Results of Uncertainty Analysis for High Level Waste Repository by FAST