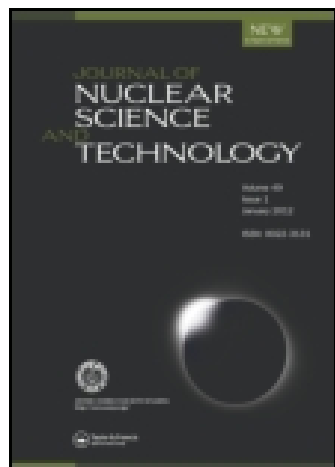


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Toshimitsu HOMMA<sup>a</sup> & Andrea SALTELLI<sup>b</sup>

<sup>a</sup> Tokai Research Establishment, Japan Atomic Energy Research Institute, Tokai-mura, Ibaraki-ken, 319-11

<sup>b</sup> Environment Institute, Joint Research Centre, European Commission, 1-21020, Ispra, VA, ITALY

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## TECHNICAL REPORT

# Use of Sobol's Quasirandom Sequence Generator for Integration of Modified Uncertainty Importance Measure

Toshimitsu HOMMA<sup>†</sup>,

*Tokai Research Establishment, Japan Atomic Energy Research Institute\*<sup>1</sup>*

Andrea SALTELLI

*Environment Institute, Joint Research Centre, European Commission\*<sup>2</sup>*

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Sensitivity analysis of model output is relevant to a number of practices, including verification of models and computer code quality assurance. It deals with the identification of influential model parameters, especially in complex models implemented in computer programs with many uncertain input variables. In a recent article a new method for sensitivity analysis, named HIM\* based on a rank transformation of the uncertainty importance measure suggested by Hora and Iman was proved very powerful for performing automated sensitivity analysis of model output, even in presence of model non-monotonicity. The same was not true of other widely used non-parametric techniques such as standardized rank regression coefficients. A drawback of the HIM\* method was the large dimension of the stochastic sample needed for its estimation, which made HIM\* impracticable for systems with large number of uncertain parameters. In the present note a more effective sampling algorithm, based on Sobol's quasirandom generator is coupled with HIM\*, thereby greatly reducing the sample size needed for an effective identification of influential variables. The performances of the new technique are investigated for two different benchmarks.

**KEYWORDS:** *sensitivity analysis, nonlinear models, non-monotonic models, quasirandom sequences, uncertainty importance measure, nonparametric estimators, Latin hypercube sampling, benchmarks, experimental data, performance, parametric analysis*

## I. INTRODUCTION

In recent analysis of model performance the use of sensitivity analysis (SA) is becoming customary. SA of model output investigates the relationship between the predictions of a model and its input parameters. This analysis is relevant to the quality assurance of models and computer codes, in what it ensures that the relation between output and input parameters is physically meaningful. It also assists in the identification of crucial regions in the parameters space, thus indicating, in the case of experimentally determinable parameters, where research effort is mostly needed. Finally SA allows the total uncertainty in model prediction to be appor-

tioned to the uncertainty in the model input parameters. In this respect SA complements Uncertainty analysis (UA), which quantifies—for instance using confidence bounds—the degree of uncertainty in model prediction.

Several SA techniques are described in the literature; a recent review is given in Helton *et al.*<sup>(1)</sup>, where the relative merits of differential analysis<sup>(2)</sup>, Fourier amplitude sensitivity test (FAST)<sup>(3)</sup> and Monte Carlo methods are discussed. A recent original work in the field of “global” SA is that of Welch *et al.*<sup>(4)</sup>,

\*<sup>1</sup> Tokai-mura, Ibaraki-ken 319-11.

\*<sup>2</sup> I-21020 Ispra (VA), ITALY.

<sup>†</sup> Present address: Institute of Nuclear Safety, Nuclear Power Engineering Corporation, Toranomon, Minato-ku, Tokyo 105.

where an efficient parameter screening based on data adaptive modeling is performed to build a computationally cheaper predictor to substitute for the original model. Another approach to SA not included in Helton *et al.*<sup>(1)</sup> is the work of Cawfield and Wu<sup>(5)</sup>, where probabilistic SA is performed within the frame of first order reliability analysis (FORM).

Inter-comparison has been made of the performances of different SA techniques<sup>(6)</sup>. More specifically in the field of Monte Carlo based global SA techniques some quantitative comparison is available<sup>(7)-(10)</sup>. An excellent theoretical discussion of global sensitivity estimates is given for nonlinear models<sup>(11)</sup>.

In most of the literature quoted above and in the present note model is considered as a black box, *i.e.* the analysis of the sensitivities is done weighting model output against model input, without assuming knowledge of model structure. This knowledge can hence be confronted critically with the results of the analysis. The analysis is also automated, in the sense that the order of importance of the relevant input parameters is done automatically based on the values of an estimator. As an example of non-automated SA visual inspection of rank scatter plot of input *vs.* output variables coupled with expert judgment could be effectively used for SA of models with few input and output variables<sup>(12)</sup>. Rank scatter plot can also be used when SA predictions from different estimators seem to contradict each other<sup>(9)(10)</sup>. Automated SA is essential for systems with many input parameters and complex time dependent or spatially dependent outputs.

This paper presents a new SA method based on modified versions of the Hora and Iman “uncertainty importance measure”<sup>(13)</sup>; two versions of this method, named HIM and HIM\* were already discussed<sup>(9)</sup>. HIM was a version of the estimator based on the raw values of the input and output vectors, while HIM\* was the rank version of the method. The reason for introducing a new estimator was the poor performance of normally reliable and robust nonparametric techniques such as standardized rank regression coefficients (SR-

RCs) and the Spearman test in presence of model non-monotonicity<sup>(9)</sup>. In those previous studies it was pointed out that the new HIM\* technique was superior to many other SA estimators as far as “reproducibility” and “accuracy” were concerned. There reproducibility was defined as a measure of how well SA predictions were replicated when repeating the analysis on different samples taken from the same input parameters space. Accuracy dealt with the physical correctness of the SA results. In discussing their version of the uncertainty importance measure Iman and Hora<sup>(14)</sup> also recognize its lack of robustness; being based on the conditional and unconditional variance of the output the measure is highly influenced by outliers associated with long tailed input distributions. Those authors suggest an alternative regression-based measure.

The increased performance of HIM and HIM\* for the test cases considered had the drawback of being computationally expensive due to the dimension of the sample size needed to compute HIM and HIM\*. Here a new sampling scheme, using Sobol’s quasirandom sequence generator<sup>(15)-(18)</sup> has been attempted, which allows a drastic reduction in the sample size, thus upgrading the performance of these estimators. The performance of HIM and HIM\* with the new sampling scheme is tested against two benchmarks; the first one is a case where an analytical (and hence exact) evaluation of HIM is possible; the second one is a more complex test case where the integration of HIM\* can only be done numerically. Crude Monte Carlo (CMC) sampling and Latin hypercube sampling (LHS) have been compared with the approach based on Sobol’s  $LP_\tau$  sequences. The similarities between HIM and a sensitivity measure  $S_j$  proposed by Sobol’<sup>(11)</sup> are also highlighted.

## II. METHODS

The importance measure discussed in this article was initially proposed as a sensitivity analysis method by Hora and Iman<sup>(13)</sup>. It was then made computationally more effective by Ishigami and Homma<sup>(19)(20)</sup> and further mod-

ified by Saltelli *et al.*<sup>(9)</sup>

The uncertainty importance measure given by Hora and Iman<sup>(13)</sup> focuses on the contribution to the variance of the model output attributable to the uncertainty in each of the model input variables. Let the output variable  $Y$  be a function of  $K$  variables

$$Y = h(X_1, X_2, \dots, X_K), \quad (1)$$

The variance of  $Y$ ,  $\text{Var}(Y)$  can be reduced if the value of an input variable,  $X_j$  is known with certainty. The conditional variance of  $Y$ ,  $\text{Var}(Y|X_j)$  is the reduced variance and thus  $\text{Var}(Y) - \text{Var}(Y|X_j)$  is the conditional reduction in the variance of  $Y$  attributable to ascertaining the “fixing” of the input  $X_j$ . The dependence of the conditional variance  $\text{Var}(Y|X_j)$  upon the specific value  $\tilde{x}_j$  can be eliminated by averaging over the possible values of the fixed variable. Thus they defined the measure of uncertainty importance as the square root of the expected reduction in the variance of  $Y$  attributable to ascertaining the value of  $X_j$ <sup>(13)</sup>:

$$I_j = \sqrt{\text{Var}(Y) - E[\text{Var}(Y|X_j)]}. \quad (2)$$

This can be also written as<sup>(19)</sup>

$$I_j = \sqrt{U_j - \langle Y \rangle^2}, \quad (3)$$

where  $\langle Y \rangle$  is the mean of the output and

$$U_j = \int \langle h(\tilde{x}_j) \rangle^2 f_j(\tilde{x}_j) d\tilde{x}_j, \quad (4)$$

$\langle h(\tilde{x}_j) \rangle$  is the mean of  $Y$  when the variable  $X_j$  is fixed to the value  $\tilde{x}_j$ , and  $f_j(\tilde{x}_j)$  is the probability density function of variable  $X_j$ .  $X_j$  ( $j=1, 2, \dots, K$ ) is considered to be distributed in a pre-determined range. All variables  $X_1, \dots, X_K$  are assumed to be independent.

If now  $I_j$  is used to rank the influence of each input parameter  $X_j$  on the output variable  $Y$ , the variable ranking will in fact be based on the values of  $U_j$ , *i.e.* variable  $k$  will be more important than variable  $j$  if  $U_k > U_j$ .

The problem of estimating  $U_j$  through Monte Carlo computations has been addressed in Ishigami and Homma<sup>(19)</sup>, where a

modified version of the estimator was defined as the scalar product

$$\text{HIM}(X_j) \doteq \frac{1}{N} \mathbf{Y}_B \cdot \mathbf{Y}_j = \frac{1}{N} \sum_{i=1}^N y_i y_i^j. \quad (5)$$

In this formula the two output vectors  $\mathbf{Y}_B \equiv (y_1, \dots, y_N)$  and  $\mathbf{Y}_j \equiv (y_1^j, \dots, y_N^j)$  contain the outcome of two independent sets of Monte Carlo simulations of size  $N$ . The  $y_i, y_i^j$  values are computed based on two independent input data matrices, one denominated “base” and one “new”, both of the same size  $N$ . Only one base vector  $\mathbf{Y}_B$  is computed for all the variables from “base”; for each variable  $X_j$  then the  $\mathbf{Y}_j$  vector is computed from an input matrix whose columns are all from “new” but for column  $j$ , from “base”<sup>(9)</sup>. In this way the input matrices for two generic variables  $X_j$  and  $X_k$  now only differ for columns “ $j$ ” and “ $k$ ”. Beside minimizing the noise associated to the measure this technique reduces the number of model evaluations to  $N \times (K+1)$ .

The above scheme for SA was tested for accuracy and reproducibility against a number of other sensitivity analysis estimators including Spearman and SRRC<sup>(9)</sup>. Reproducibility was investigated by repeating the SA on different input samples from the same distributions and computing the variance in the methods prediction. The reproducibility of HIM was found to be poor; the summation in Eq.(5) is very sensitive to distribution outliers, especially when the values of the output function  $Y$  range over several orders of magnitude. The analysis was then repeated by replacing the  $y_i^j, y_i$  values in Eq.(5) by their ranks:

$$\text{HIM}^* \doteq \frac{1}{N} \sum_{i=1}^N R(y_i) R(y_i^j). \quad (6)$$

For non-influential variables  $\text{HIM}^*$  will tend to

$$(\text{HIM}^*)_{\min}^* \approx \left( \frac{N+1}{2} \right)^2; \quad (7)$$

for influential variables (perfectly correlated  $R(y_i), R(y_i^j)$ )  $\text{HIM}^*$  will tend to

$$(\text{HIM}^*)_{\max}^* = \frac{1}{N} \sum_{i=1}^N i^2 = \frac{(N+1)(2N+1)}{6}. \quad (8)$$

A convenient scaling for  $\text{HIM}^*$  which has been adopted in the present work is then:

$$\begin{aligned} \text{HIM}^* &\stackrel{\text{(Eq.(6))}}{\text{replaced by}} \frac{(\text{HIM}^* - (\text{HIM}^*)_{\min})}{(\text{HIM}^*_{\max} - (\text{HIM}^*)_{\min})} \\ &= \frac{\left[ \frac{1}{N} \sum_{i=1}^N R(y_i) R(y_i^j) - \left( \frac{N+1}{2} \right)^2 \right]}{\left( \frac{N^2 - 1}{12} \right)}, \quad (9) \end{aligned}$$

whereby  $\text{HIM}^*$  is bound between 0 (loosely) and 1 (tightly). The new estimator, indicated as  $\text{HIM}^*$  was both accurate and reproducible, yielding correct ranking of model sensitivities even in presence of model non-monotonicities, a feature which affected negatively other robust SA estimators such as the SRRCs, the partial rank correlation coefficients (PRCC), the Spearman test and the like. It must be noted that in this formulation the  $\text{HIM}^*$  estimator coincides (even computationally) with a sensitivity measure  $S_j$  suggested by Sobol'<sup>(11)</sup>.

$$S_j \doteq \frac{\left[ \frac{1}{N} \sum_{i=1}^N y_i y_i^j - f_0^2 \right]}{\left[ \frac{1}{N} \sum_{i=1}^N (y_i)^2 - f_0^2 \right]}, \quad (10)$$

where

$$f_0^2 \doteq \frac{1}{N} \sum_{i=1}^N y_i. \quad (11)$$

If we replace in Eqs.(10) and (11) the raw data with the rank-transformed data we obtain our Eq.(9) after some algebra.

One shortcoming of the importance measures  $\text{HIM}$ ,  $\text{HIM}^*$  (and  $S_j$ ) when compared with the regression/correlation based estimators such as SRRC, PRCC is that the former still requires  $N \times (K+1)$  model evaluations as compared to the  $N$  needed to compute either PRCC or SRRC. This makes the possibility of using  $\text{HIM}$  and  $\text{HIM}^*$  very much dependent on the number of variables in the model. In order to further reduce the sample size needed to compute  $\text{HIM}$  and  $\text{HIM}^*$  in the present note an alternative sampling scheme is attempted, replacing CMC used in the previous analyses with quasirandom sequences generated according to an algorithm proposed by Sobol'<sup>(21)</sup>.

Quasi-Monte Carlo methods, the deterministic versions of Monte Carlo techniques, have the widest applications in numerical integration. Let us consider the Monte Carlo approximation of integrals over a  $s$ -dimensional unit cube  $I_s = [0, 1]^s$ .

$$\int_{I^s} f(x) dx \approx \frac{1}{N} \sum_{n=1}^N f(P_n), \quad (12)$$

where a set of points  $P_n$  ( $n = 1, \dots, N$ ) belongs to  $I^s$ . The idea of a quasi-Monte Carlo method is that one may use uniformly distributed sequences in place of random points in order to improve the expected integration error  $O(N^{-1/2})$ .

The concept of "discrepancy" must be defined here. For a set of  $N$  points in  $I^s$  can be defined as<sup>(22)</sup>:

$$D_N^{(s)} = \sup_J \left| \frac{A(J; N)}{N} - \text{Vol}(J) \right|, \quad (13)$$

where the supremum is extended over the rectangular  $s$ -dimensional region:

$$J = [0, x_1] \times [0, x_2] \times \dots \times [0, x_s] \quad (14)$$

with volume  $x_1 x_2 \dots x_s$ .  $A(J; N)$  is defined as the number of points in  $J$  and  $\text{Vol}(J)$  is volume of  $J$ . Estimates for integration errors can be established in terms of the following Koksma-Hlawka inequality:

$$\left| \int_{I^s} f(x) dx - \frac{1}{N} \sum_{n=1}^N f(P_n) \right| \leq V(f) D_N^{(s)}, \quad (15)$$

where  $V(f)$ , which is called a function of bounded variation in the sense of Hardy and Krause, indicates the regularity of the integrand<sup>(22)</sup>. It is known that there exists a finite sequence of  $N$  points in  $I^s$  such that:

$$D_N^{(s)} = O((\log N)^{s-1}/N). \quad (16)$$

Thus quasi-Monte Carlo integration with determinate low-discrepancy sequence involves effective error bounds that are considerably smaller than the Monte Carlo bound  $O(N^{-1/2})$ . Sequences that aim for low discrepancy are called quasirandom.

Several ways of generating such sequences are known<sup>(23)(24)</sup>. A description of how those sequences are generated is given in Bratley and Fox<sup>(18)</sup>, where the performances of two quasirandom sequence generators for a set

of numerical integrations at different sample sizes are compared. For the present work Sobol's FORTRAN code LPTAU<sup>(21)</sup> was used. All  $LP_\tau$  sequences suggested by Sobol' satisfy the following conditions:

- (a) the uniformity of the distribution should be asymptotically optimal,
- (b) uniformity of the points should be observed not only as  $N \rightarrow \infty$ , but also for fairly small  $N$  (for  $n \leq 16$ ) and
- (c) the algorithm for computing the points should be fairly simple (for  $n \leq 51$ ).

LPTAU was coupled with the PREP code<sup>(25)</sup>. PREP also generates the CMC sample and Latin hypercube sample (LHS) needed for the comparison and converts those unit cube values to the values needed in the actual input distributions. The first testing of Sobol' sampling was done on the numerical integration of a function in Ishigami and Homma<sup>(19)</sup> where an analytical expression is also available for HIM. The second test is done directly on HIM\* using a model already used in Saltelli *et al.*<sup>(9)</sup> This latter was computed using the LISA code<sup>(26)</sup>.

### III. APPLICATIONS

#### 1. Application of Quasirandom Sequences to HIM Estimator

In order to examine the accuracy and reproducibility of Sobol' quasirandom sequences in computing an estimate of the integral in Eq.(4), the following analytical function is used:

$$h(X_1, X_2, X_3) = \sin X_1 + a \sin^2 X_2 + b X_3^4 \sin X_1. \quad (17)$$

If the probability distribution functions (pdf) for each variable  $X_j$  are given by

$$f_i(X_i) = \begin{cases} \frac{1}{2\pi}, & \text{when } -\pi \leq X_i \leq \pi \\ 0, & \text{when } X_i < -\pi, X_i > \pi \end{cases} \quad (18)$$

for  $i = 1, 2, 3$ ,

then the exact value of  $U_j$  ( $j=1, 2, 3$ ) in Eq.(4) can be obtained analytically as:

$$U_1 = \frac{a^2}{4} + \left(1 + \frac{b\pi^4}{5}\right)^2 / 2, \quad (19)$$

$$U_2 = \frac{3a^2}{8}, \quad (20)$$

$$U_3 = \frac{a^2}{4}. \quad (21)$$

As  $HIM(X_i)$  is an estimator of  $U_j$  ( $j=1,2,3$ ), the evaluation of Eq.(5) using quasirandom sequences can now be compared with those exact values. The function used here has characteristics of strong non-linearity and non-monotonicity. Parametric and nonparametric techniques based on regression/correlation measures (*e.g.* Superman, SRRC) were proven ineffective in ranking the relative importance of the input parameters for this model<sup>(20)</sup>.

In order to compute  $HIM(X_j)$ , a unit cube in the  $2K$  dimensional space is assumed, where  $K$ , number of independent variables, is three in this case.  $N$  points are selected in this cube by the Sobol' algorithm, thereby generating a matrix of size  $(N, 2K)$ . The first  $K$  columns of this matrix are used to produce the "base" matrix and the remaining columns are used as the "new" matrix (see Chapter II). Table 1 shows the comparison of  $HIM(X_j)$  values calculated by the Sobol' sampling scheme for different sample sizes with the exact values. The constants in Eqs.(19) to (21) are given the values  $a=7$  and  $b=0.1$ . Table 1 also provides an estimate for the mean square error in the estimator  $HIM(X_j)$  of Eq.(5). As can be seen from Table 1, this scheme yields the precise estimates for large enough sample sizes, and also provides a good performance even at the smaller sample sizes.

The good performance of Sobol' method is confirmed by comparing the variability of  $HIM(X_j)$  integrated by Sobol' method with that integrated *via* CMC or LHS at different sample sizes. This is done as follows:

- 1) For each sample sizes  $N$  ranging between 16 ( $=2^4$ ) and 1024 ( $=2^{10}$ ) the CMC and LHS calculations of  $HIM(X_j)$  are repeated one hundred times, changing each time the seed for the random number generation. For Sobol' method, 100 independent groups of  $N$  sample sizes are

**Table 1** Convergence of  $HIM(X_i)$  calculated by Sobol' method

Sample size	$HIM(X_1)$	MSE	$HIM(X_2)$	MSE	$HIM(X_3)$	MSE
16	12.174	4.782	16.222	4.726	11.446	4.288
32	20.302	5.445	17.480	3.267	12.017	4.115
64	17.885	3.707	19.065	2.285	13.340	2.508
128	16.446	2.341	18.548	2.101	13.527	2.390
256	16.649	1.581	17.761	1.451	12.184	1.685
512	16.756	1.127	17.982	1.078	12.437	1.172
1024	16.678	0.789	18.275	0.770	12.315	0.830
2048	16.652	0.562	18.315	0.568	12.313	0.577
4096	16.590	0.397	18.314	0.402	12.254	0.409
Exact	16.596		18.375		12.250	

selected from  $LP_\tau$  sequences. For each sample size, 100 different evaluations of  $HIM(X_1)$ ,  $HIM(X_2)$  and  $HIM(X_3)$  are produced.

- 2) The difference between each  $HIM(X_j)$  evaluation and the analytical value is computed.
- 3) For each sample size  $s_i$ , sampling scheme (scheme=CMC, LHS and Sobol') and variable  $X_j$  the estimate of the mean square error MSE of the differences over the 100 samples is computed:

$$\Delta_{\text{scheme}}^{\text{MSE}}(X_j, s_i), \text{ scheme} = \text{CMC, LHS, Sobol'}, j = 1, 2, 3, s_i = 2^4, \dots, 2^{10}$$

$$= \text{MSE of } [HIM_m(X_j, s_i) - HIM_{\text{analyt.}}(X_j)] \text{ over 100 evaluations. (22)}$$

Those MSE's are given in **Table 2**. It can be seen that the mean square errors associated with the evaluation done *via* Sobol' are almost always lower than those associated with both CMC and LHS. For instance, the evaluation by Sobol' method at sample size, 256 already provides better performance than those with both CMC and LHS at sample size, 1024. The performances of CMC and LHS are very similar over the entire sample sizes. As pointed out by McKay *et al.*<sup>(27)</sup> the superiority of LHS with respect to CMC can only be proved for monotonic functions. For the strong non-monotonic test function used here there appears to be no benefit in using LHS rather than CMC. Stein<sup>(28)</sup> proves LHS's asymptotic superiority even for non-

**Table 2** Comparison of  $HIM(X_1)$ ,  $HIM(X_2)$  and  $HIM(X_3)$  values by three sampling schemes

Sample size	Mean square error based on 100 batches			
	CMC	LHS	Sobol'	
$HIM(X_1)$	16	4.438	4.397	5.982
	32	3.111	3.012	2.422
	64	1.595	2.030	1.654
	128	1.363	1.295	0.463
	256	0.974	0.920	0.153
	512	0.678	0.757	0.069
1024	0.455	0.500	0.055	
$HIM(X_2)$	16	4.384	4.422	5.166
	32	2.980	2.899	3.033
	64	2.183	2.026	1.090
	128	1.341	1.413	0.795
	256	1.007	0.953	0.400
	512	0.643	0.722	0.375
1024	0.399	0.481	0.092	
$HIM(X_3)$	16	5.984	6.715	5.133
	32	3.870	3.733	3.346
	64	2.739	2.554	1.601
	128	1.852	1.714	1.416
	256	1.320	1.254	0.292
	512	0.884	0.857	0.090
1024	0.654	0.611	0.072	

monotonic models. Far from the asymptote, and for the strong non-monotonic test function used here, Sobol' method gives the great reduction of the sample size needed for the estimates of  $HIM(X_j)$ .

## 2. Application of Quasirandom Sequences to $HIM^*$ Estimator

As pointed out in Saltelli *et al.*<sup>(9)</sup>  $HIM^*$  is characterized by an enhanced reproducibil-

ity with respect to HIM and hence is to be preferred when performing SA on samples of limited size for computationally expensive models.

The test case employed here was already discussed in the above article. The detailed description of the model, named Level E, was given there and also in the OECD/NEA report<sup>(29)</sup>; only its essential features are repeated here. The test model involves the computation of the dose to man resulting from migration of four radionuclides:  $^{129}\text{I}$  and the  $^{237}\text{Np}$ - $^{233}\text{U}$ - $^{229}\text{Th}$  chain through a multi-barrier system (waste form, geosphere, biosphere). The resulting doses are obtained by convoluting the source terms with the responses of the geosphere and multiplying by a biosphere dilution term and by the radiological exposure factors. The geosphere model includes a two layer path length where dispersion, advection, chemical retention and radioactive decay have to be modeled. Only uniform type distributions on both linear and logarithmic scale are considered for the twelve input distributed parameters.

The mean output (dose rate) from a simulation of size 1024 is shown as a function of time in Fig.1, where the first peak of the total dose is due to the  $^{129}\text{I}$  contribution and the second one due to the  $^{237}\text{Np}$  chain. In

Fig.2 the model coefficients of determination  $R_y^2$  are given for the total dose summed over all the radionuclides. Those coefficients are computed from the regression models based on the raw values and the ranks. This coefficient provides a measure of how well the linear regression model based on either the standardized regression coefficients (SRC's) or SRRC's can reproduce the actual output vector. As can be seen in Fig.2,  $R_y^2$  based on the raw values are always low. The large difference between the values of these two coefficients demonstrates the non-linearity of the model. This indicates that a SA based on linear estimators like SRC and the Pearson test is inadequate. As shown in Saltelli *et al.*<sup>(9)</sup>, the multi-modal shape of the  $R_y^2$  curve based on the ranks suggests that – close to the local minima of the curve – even the nonparametric estimators may fail to identify the influential parameters. In effect inspection of rank scatter plots revealed that those minima corresponded to region where the dose and input parameter relationship was non-monotonic. Among the nonparametric estimators only HIM\* could correctly identify the most influential parameter, which is the water velocity in the first layer of the geosphere (FLOWV1, Fig.3).

In order to compare the performance of

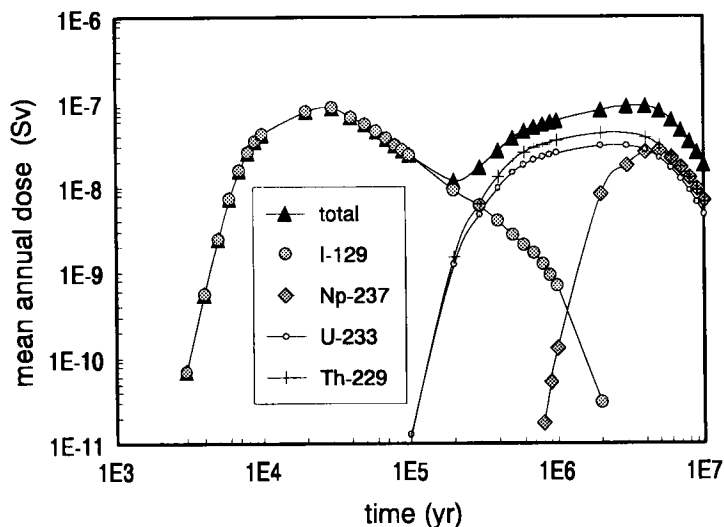


Fig.1 Mean annual dose (Sv) for the radionuclides considered in Level E test case as function of time



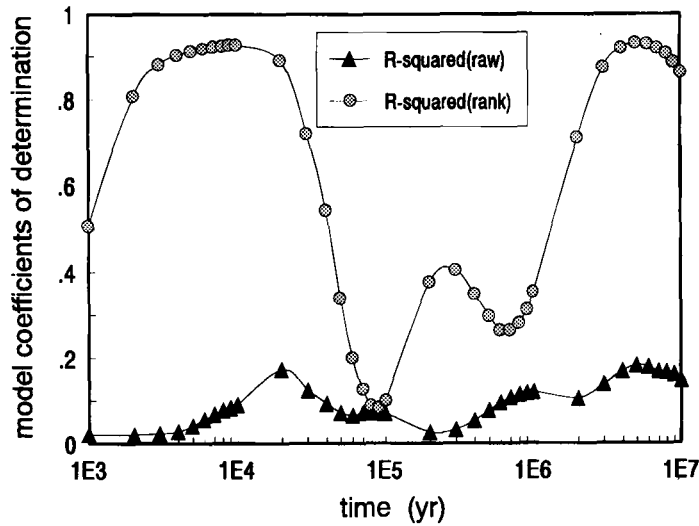


Fig.2 Model coefficients of determination ( $R_y^2$ ) on raw values and ranks for Level E test case

sampling schemes in computing HIM\* an alternative must be found to the use of the exact analytical solutions, which are not available for this test case. As a replacement two “large” samples of size 1024 are produced *via* CMC and Sobol’ to be used as a reference. **Figure 3** shows  $HIM^*(X_j, t)$  as computed from a sample of size 1024 *via* Sobol’ for all the input parameters  $X_j$ . Figure 3 shows that

FLOWV1 (flow velocity in the first tract of the geosphere path) is by far the most important variable, apart from some early time points where PATHL1 (length of the same tract) predominates. At late time points some influence is evident of the variable RETF1C, linked to the chemical retention of the radionuclides in the  $^{237}\text{Np}$  chain.

The performances of Sobol’ and CMC

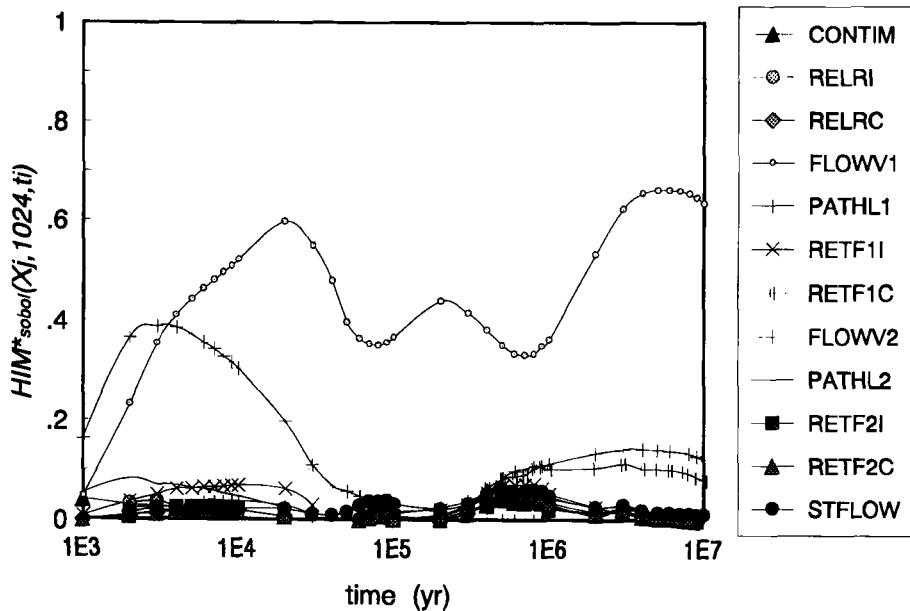


Fig.3  $HIM^*$  curve for Level E variables as function of time

methods for those three influential variables are compared at various sample size. First the difference:

$$\Delta_{\text{CMC}}(X_j, s_i, t_i) = \text{HIM}_{\text{CMC}}^*(X_j, s_i, t_i) - \text{HIM}_{\text{CMC}}^*(X_j, 1024, t_i) \quad (23)$$

and the analogous  $\Delta_{\text{Sobol}}(X_j, s_i, t_i)$  for Sobol' sampling are calculated as a function of time. Due to the computational cost of this test case smaller batches are used for the various sample sizes, *i.e.*

4 batches of size 256;

8 batches of size 128;

16 batches of size 64;

32 batches of size 32.

Those batches allow  $\Delta_{\text{CMC}}^{\text{MSE}}(X_j, s_i, t_i)$  to be computed. For economy of plots the time dimension is eliminated by averaging the SA results over all the different time points  $t_i$  to yield  $\bar{\Delta}_{\text{CMC}}^{\text{MSE}}(X_j, s_i)$ , where the bar stands for average. A similar averaging is done for the Sobol' batch samples, to yield  $\bar{\Delta}_{\text{Sobol}}^{\text{MSE}}(X_j, s_i)$ . The results are presented in **Table 3** for the three most influential variables. The advantage of using Sobol' is evident.

#### IV. CONCLUSIONS

The starting point of the present investigation was the proven inadequacy of rank based nonparametric techniques (PRCC, SRRC, ...) to provide a measure for automated SA of complex models. Complexity in this context does not refer particularly to the number of equations involved, but rather to the existence of non-linearity and non-monotonicity in the output functions dependent from the input variables (a frequent occurrence in modelling). The HIM\* method, resulting from an upgrade of existing tech-

niques, was proved to be adequate for the purpose of automated SA. HIM\* was proved to be very reproducible and accurate, even in presence of model complexity. One drawback of this estimator is the dependence of the total number of model evaluations to be used in the investigation upon the number of uncertain variables, *i.e.*

$$N_{\text{TOT}} = N \times (K + 1), \quad (24)$$

where  $N$  is the sample size needed to compute HIM\* for any variable and  $K$  the number of variables. For computationally expensive models then the possibility of using HIM\* for SA is limited by the number of variables in the model. The present article has shown that the use of Sobol' quasirandom sequences results in a great reduction of the sample size  $N$  needed to compute HIM\* without loss of accuracy, thereby enlarging the class of models for which the HIM\* approach is applicable.

For the extreme case of complex models with large number of uncertain parameters, a detailed SA with HIM\* could still be worth being pursued once a preliminary screening of the parameters is done. A screening technique which was proven very effective is the iterated fractional factorial design (IFFD), capable identifying few influential parameters in models with several hundreds of input variables<sup>(10)</sup>.

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**Table 3** Comparison of mean square error by two sampling schemes

Sample size	FLOW1		PATHL1		RETF1C	
	CMC	Sobol'	CMC	Sobol'	CMC	Sobol'
32	0.140	0.113	0.169	0.139	0.169	0.136
64	0.098	0.065	0.126	0.074	0.123	0.076
128	0.065	0.037	0.066	0.051	0.075	0.046
256	0.046	0.027	0.037	0.029	0.059	0.028

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