

**KfK 4626
Juni 1990**

Procedures for Uncertainty Analyses of UFOMOD A User Guide

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**PROCEDURES FOR UNCERTAINTY
ANALYSES OF UFOMOD
- A USER GUIDE -**

F. Fischer

Work has been performed with support of the
Commission of the European Communities
Radiation Protection Programme
Contract No. BI6/F/128/D

Kernforschungszentrum Karlsruhe GmbH, Karlsruhe

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Kernforschungszentrum Karlsruhe GmbH
Postfach 3640, 7500 Karlsruhe 1

ISSN 0303-4003

Abstract

This user guide describes the procedural steps and some necessary mathematical background information for uncertainty analyses performed with the accident consequence assessment code UFOMOD. As an example the countermeasures submodule of UFOMOD, Version NE 87/1, has been chosen, on one hand to demonstrate the various steps of an uncertainty and sensitivity analysis and on the other hand to show the application of the supporting mathematical tools such as codes for generating the experimental design, calculating confidence bounds and quantifying sensitivity measures like partial rank correlation coefficients (PRCCs) and coefficients of determination, R^2 .

Examples of input and output of the uncertainty codes and the graphics program are given, which shows the complementary cumulative frequency distributions (CCFDs) of consequences and their variability.

This user guide shall complement, but not substitute, the corresponding detailed user guides of the original uncertainty codes.

Prozeduren für Unsicherheitsanalysen zum Programmsystem UFOMOD - Eine Benutzeranleitung -

Diese Benutzeranleitung beschreibt die prozeduralen Schritte und in einem gewissen Umfang den notwendigen mathematischen Hintergrund zu Unsicherheitsanalysen für das Unfallfolgen - Programmsystem UFOMOD. Als Beispiel wurde der Schutz- und Gegenmaßnahmen - Teilmodul des Programmsystems UFOMOD, Version NE 87/1, ausgewählt, um daran einerseits die verschiedenen notwendigen Schritte bei Unsicherheits- und Sensitivitätsuntersuchungen zu demonstrieren und andererseits die Anwendung von unterstützenden mathematischen Werkzeugen wie Computer - Codes zur Erstellung eines statistischen Versuchsplans, zur Abschätzung von Konfidenzbändern und zur Quantifizierung von partiellen Rangkorrelationskoeffizienten (PRCCs) oder Bestimmtheitsmaßen, R^2 , zu erläutern.

Es werden Beispiele für Eingabe und Ausgabe der Unsicherheitsanalysen - Codes gegeben wie auch für das zugehörige Graphik - Programm, das die komplementären kumulative Häufigkeitsverteilungen (CCFDs) der Konsequenzvariablen und deren Variabilität beschreibt.

Diese Benutzeranleitung soll die Benutzeranleitungen der originalen Unsicherheitsanalyseprogramme ergänzen, aber nicht ersetzen.

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1. Introduction

During the last years uncertainty analysis investigations were performed at KfK within the within the CEC - MARIA¹ programme (see [24]), aiming at an enhancement of applicability, efficiency and reliability of several techniques available for uncertainty analysis of large computer models.

There exists a considerable variety of such methods, with wide difference in conceptual approach, computational effort required, and the power of their results. Clearly, no one method is always best; the choice should depend both on the nature of the problem and the resources available to the analyst.

This report refers to an uncertainty analysis of a submodule of the program system UFOMOD, version NE87/1. It should serve as a guideline how to use uncertainty/sensitivity procedures available at KfK. For a detailed submodule description of UFOMOD and the corresponding uncertainty analyses, its interpretations and conclusions the reader is referred to [7] and [9], respectively.

In this study the notion of uncertainty analyses is used in the general sense of investigation of model predictions under conditions of parameter variability and focusses on

- the estimation of confidence bounds for consequences, which show how much variability exists, and
- sensitivity measures, which examine relationships between changes in consequences due to changes in model parameter² values and provide a ranking of importance.

Some general features which are important in performing uncertainty analyses for accident consequence models like the program system UFOMOD, are described in Chap. 2.

Chapter 3 comprises the procedural actions for uncertainty analyses. As an example the countermeasures submodule of UFOMOD is chosen.

Having defined ranges and distributions for model parameters (Chapter 3.1) it is necessary to select specific values for each of the uncertain model parameters to be used in each run of UFOMOD, i.e. to have a suitable sampling scheme. For a sampling scheme to be effective

¹ CEC : Commission of the European Communities
MARIA: Methods for Assessing the Radiological Impact of Accidents
within the CEC Radiation Protection Research Programme

² In this study, the wording '*model parameters*' comprise '*parameters*' and some '*input variables*' of submodules of UFOMOD

the generated model parameter values should adequately span the model parameter space. The Latin hypercube sampling (LHS) procedure in contrast to the well-known random sampling design (RSD) forces the entire range of each model parameter to be sampled. In Chapter 3.2 the LHS - sampling scheme and the IMAN/CONOVER - procedure (see [14]) for inducing rank correlations is indicated.

Each UFOMOD run produces *one* complementary cumulative frequency distribution (CCFD). Chapter 3.3 briefly describes the estimation of confidence bounds for CCFDs. The width of the band is an indicator of the sensitivity of model predictions with respect to variations in parameters, which are imprecisely known.

To quantify the relative importance of the uncertain model parameters to the output of the accident consequence model some sensitivity measures are needed to 'rank' the parameters with respect to their influence on the consequences. This will be explained in Chapter 3.4.

The partial (rank) correlation coefficient PCC or PRCC, respectively, are measures that quantify the relation between a consequence variable and one or more model parameters. When a nonlinear relationship is involved it is often more revealing to calculate PCCs between variable *ranks* than between the *actual* values for the variables. The numerical value of the PRCCs can be used for hypothesis testing to quantify the confidence in the correlation itself, i.e. by statistical reasons one can determine which PRCC values indicate really an importance (significance) of a parameter or which PRCC values are simply due to 'white noise'. Moreover, it is possible to calculate the percentage contribution of each uncertain model parameter to uncertainty in consequences by use of so-called *coefficients of determination* (R^2).

The last step in performing uncertainty analyses is to present and interpret the results of the analyses.

2. General Features

An uncertainty analysis of ACA - model predictions is a systematic procedure to quantify - by means of mathematical tools - limits within which reality is expected to lie. Determining the sources and the extent of uncertainties takes in aspects of data collection, development of methods and presentation of results.

In probabilistic consequence assessments the impact of an accidental release of radioactive materials to the environment is described by a variety of accident consequences. The frequencies or probabilities of these consequences are estimated and the results are presented in form of frequency distributions (complementary cumulative frequency distributions, CCFDs).

The frequency distributions give an indication of the variability in the real world and of the unpredictability of the environmental conditions. Because of the lack of experimental data the assumptions, models and data in an ACA include a good deal of engineering assessment and subjective judgement. This gives a certain degree of inaccuracy or uncertainty. There are several sources of uncertainty. Firstly there are *modelling uncertainties*, which may exist due to inadequate mathematical formulation of physical phenomena. Secondly there are *completeness uncertainties*, which may result from the fact, that contributions to risk have not been considered comprehensively. Thirdly there are *uncertainties in parameter values* due to lack of knowledge about the best value to use in an assessment. They must be clearly distinguished from the uncertainty due to physical variability in environmental conditions, expressed by random variables. The influence on the results of an accident consequence assessment is quite different for the two cases. While the second type of uncertainties (e.g. unknown weather conditions during release) leads actually to the desired results of the probabilistic assessment (namely the frequency distributions of consequences), the first type causes uncertainties in these results and is in general quantitatively expressed by so-called 'confidence bands' of the frequency distributions.

What differentiates physical variability from 'lack of knowledge' - uncertainty (i.e. the parameters are fixed, but with unknown values) is the impact that additional knowledge has. As we gain more knowledge, uncertainty will decrease; however physical variability will not decrease (e.g. unpredictability of weather conditions). Nevertheless a numerical assessment of that variability can be made in a more precise manner. We will know parameter values better in modeling (e.g. deposition velocities in atmospheric dispersion and deposition calculations) and be able to quantify them more precisely; however, the variability (e.g. caused by 'rain' or 'no rain') itself will not diminish (see [3], [11]).

Identification of sources of uncertainty is not the only problem in an ACA. Usually accident consequence models are combinations of various complex submodels with a lot of uncertain

model parameters, e.g. the atmospheric dispersion and deposition submodel, the protective action submodel, the dosimetry submodel, the health effects submodel. Computer codes are being constructed to help analysts to describe complex physical phenomena and their interdependencies. The output of these commonly long - running codes like UFOMOD has to be studied with uncertainty analyses under the condition of model parameters or input values which are not well - known.

From these statements, following [1] or [2] , an uncertainty analysis is performed in the following steps:

1. Identification of model parameters thought to contribute to uncertainty in model predictions.
2. Estimation of upper and lower bounds for each 'uncertainty relevant' parameter over its assumed range, definition of distributions and estimation of correlations between model parameters.
3. Stratified sampling from the estimated distributions of the input parameters.
4. Accident consequence assessments with the sampled parameter values.
5. Estimation of consequence distribution functions to determine the variation in consequences that result from the collective variation in input parameter values.
6. Examination of relationships between parameters and consequences to determine the change in the response of the computer model to changes of individual parameters values.
7. Presentation and interpretation of the results of the analysis.

These tasks will now be explained in more detail.

1. Identification of uncertain model parameters

Based on a detailed knowledge about the underlying physical processes in an accident consequence assessment it should be possible to identify sources of uncertain model parameters. Sometimes it is useful, on one hand, to *screen out* carefully groups of parameters from further analysis, because it is clear in advance that they are unimportant with respect to the analysis. On the other hand, the *aggregation* of parameters helps to reduce the often tremendous amount of calculations and to identify model components which seem to have a large potential for contributing to uncertainty or are of minor importance.

2. Characterization of uncertain model parameters

This most important step should be done in thorough discussion with model experts to get a commonly agreed statements about the characteristics of the uncertain model parameters:

- the conceivable **range of values** (or upper/lower bounds of values)
- **the type of distribution**

Following [27], in the case of minimum knowledge, the distribution should be uniform over the conceivable range. If there exists additional expert knowledge it will possibly lead to distributions that are either unimodal and symmetric (e.g. triangular) or are skewed to the lower or higher end of the range. For large ranges it is usually preferable to choose logarithms of parameter values and to fit a uniform, triangular or normal distribution to the logarithms (i.e. loguniform, logtriangular and lognormal distributions for the parameter values). But keep in mind: Often even experts have problems to justify very large endpoints e.g. in lognormal distributions. So it is better to find adequate truncation points to cut the distribution at specified endpoints. In [1] it is pointed out that estimated distribution functions of the consequence variables can only be meaningful interpreted in a probabilistic sense if the uncertain model parameters have meaningful probability distributions associated with them. This is easy to state, but experimental data can be found scarcely to justify the chosen probability distributions. So we add a further statement: Our chain is as strong as its weakest link: data base.

In view of sensitivity analyses, it is mentioned in [1] that to determine those model parameters that contribute significantly to uncertainty, the probabilistic form of the distribution is not as important as is the representation of each parameter over its entire physically possible range.

- **correlations**

Correlations are also assumed to reflect expected restrictions or dependencies between several uncertain model parameters. Depending on how well grounded the knowledge about restrictions on the underlying parameters is you may use *no correlations* (random pairing of parameters during sampling) or *induced rank correlations* (restricted pairing of parameters during sampling).

Remark:

For the purpose of clearness almost all uncertain parameters will be split into two factors: $Par = w \cdot Par_{ref}$ the first of them, w , being a (in some way 'standardized') random variable with a suitable frequency distribution, and the second one being the best estimate or reference value of the corresponding model parameter. The reason is to decouple the discussion about the 'best' reference value from the construction of the sampling plan or design.

□

3. Sampling from the distributions of model parameters

For a sampling plan or scheme to be effective the generated model parameter values should adequately span the model parameter space. In a *Latin hypercube sample* the range of each uncertain model parameter is stratified into 'n' nonoverlapping intervals on the basis of equal probability. From each of these intervals a value is selected randomly. This process is repeated for each of the 'k' uncertain model parameters. Each selected sample makes a

column in a $n \cdot k$ sampling matrix. Then the elements in each column are randomly mixed. In contrast to the traditional random sampling the LHS - method forces the entire range of each model parameter to be sampled.

The SANDIA - LHS program [17], which is used at KfK generates samples due to traditional simple random sampling (Monte Carlo sampling), restricted random sampling (i.e. correlated parameters have to be considered), simple Latin hypercube sampling (without induced correlations) and restricted Latin hypercube sampling.

Hints:

If there is enough computer time test the following:

- Lead different samples of the same sample size to nearly identical frequency distributions of the ACA consequence variables ?
A negative answer forces to increase the sample size and to run the ACA - code again. Our experience shows that sample sizes of 1.5 times the number of model parameters are sufficient for the estimation of CCFDs of consequence variables. (To get statistically stable results for sensitivity analyses, larger sample sizes are needed, as will be indicated later.)
- Compare the effects on the frequency distributions of the consequences with respect to the same sample size of different sampling schemes (random sampling or LHS). The larger the sample size the smaller the distinction between random sampling and LHS.
- Check distribution effects in the LHS - code. For some model parameter distribution types (e.g. lognormal distributions) there are differences between raw and rank values in the correlation matrices of the LHS - code. Try to avoid sophisticated distributions or approximate them by a linearized distribution (triangular, uniform distribution). Keep in mind that you have to argue with your experts why you have chosen simple or more complicated distributions.

4. Accident consequence assessments with the sampled parameter values

The next task is to run the accident consequence code with the sampled input parameter values from the LHS-design.

The accident consequence assessment code should have an input interface to get the sampled parameter sets (of uncertain model parameters) from the LHS - design and to run the ACA - code sequentially with the different parameter sets. There should be a well - defined output interface in the ACA - code which helps to transfer e.g. the UFOMOD - code results in the graphics program (to produce CCFDs) and to the sensitivity analysis code (to calculate sensitivity measures). It is convenient (but not absolutely mandatory) to prepare the output files already in an easy-to-use form: sets of (x,y) - values for the consequence CCFDs, i.e.

decreasing ordered y - values (relative frequency values) for increasing x - values (consequence values).

At KfK the procedure of repeatedly running the accident consequence code UFOMOD for different parameter sets was done in an automatic way.

5. Estimation of CCFDs and special curves

The following distinctions are necessary:

- There are stochastic variations e.g. in weather conditions or wind directions. Each run of UFOMOD therefore produces one frequency distribution (CCFD) of consequences.
- Due to lack of knowledge about the actual model parameter values there is an uncertainty in these results. This can quantitatively be expressed by confidence intervals of the frequency distribution of consequences.

CCFD curves are generated by considering the probability of equaling or exceeding each consequence level x_0 on the x -axis. To get confidence curves for each consequence level so-called p -quantiles are calculated from the number of n_0 of associated probability values at this consequence level. Or with other words: For each consequence level x find the ($p\%$) - smallest probability value < or the $(100 - p\%)$ smallest probability value > of n_0 ordered values, i.e. the $p \times n_0$ - or the $(1 - p) \times n_0$ -th numbers from the bottom in the ordered list of n_0 probability points. For all individual consequence levels these selected probability points are connected to obtain the estimated ($p\%$) - < or $(100 - p\%)$ > - confidence curves. For details see the example at the beginning of Chap. 3.3. In a similar manner mean-, median-, min- or max-curves can be estimated.

6. Estimation of relationships between parameters and consequences

Those uncertain input model parameters have to be identified which are important contributors to variations in consequences. Each of the uncertain model parameters is ranked on the basis of its influence on the consequences.

- Rankings beyond the first few most important uncertain parameters usually have little or no meaning in an absolute ordering, since only a few of the total number of uncertain parameters actually turns out to be significant.
- Sensitivity analysis in conjunction with any form of sampling or design is easiest to carry out *if a regression model is fitted* between the model consequences and the model parameter values. to a regression model is inherent in the calculation of correlation coefficients. But, regression techniques are influenced by extreme observations and nonlinearities. Therefore it seems to be appropriate to transform the data.

A method which is regression based, which ranks either all uncertain model parameters or only those within a subset, and which additionally avoids sophisticated transformations, is the ranking on the basis of *partial rank correlation coefficients*.

Regression analyses define the mathematical relationship between two (or more) variables, while *correlations* measure the strength of the relationship between two variables.

But do all correlation numbers indicate a significant relationship between variables, i.e. is there an actual relationship or only one by chance ('white noise')? Up to which level ('white noise'-level, **critical value**) the correlation numbers are treated as garbage?

The numerical values of correlation coefficients or partial (rank) correlations coefficients can be used for significance testing of the correlation, or with other words, for hypothesis testing to quantify the confidence in the correlation itself.

Additionally it is very useful to calculate the percentage contribution of each uncertain model parameter to uncertainty in consequences by use of the so-called *coefficients of determination*, R^2 , the ratio of explained to the total variation (in least square regression).

Experiences and hints:

- Not every PRCC value makes sense.
Therefore: Use significance tests.
- A large absolute PRCC value is not in every case an indication for a considerable amount of responsibility for uncertainty in consequences.
Therefore: Use PRCC - values *and* coefficients of determination, R^2 .
- In most cases the number of PRCCs, which are above the 'white noise level', increases with the sample size.

□

7. Presentation and interpretation of results

The last step in performing uncertainty analyses is to present and interpret the results of the analyses. I.e. you have to visualize and quantify the variations in model predictions due to uncertainty in model parameters and you have to rank the uncertain model parameters with respect to their contribution to uncertainty in consequences. So the task is interpretation of

- CCFDs and estimated confidence bands, and
- the corresponding PRCC tables including the R^2 contribution

The extent and kind of presentation is clearly influenced by the central points of interest the model experts and decision - makers have.

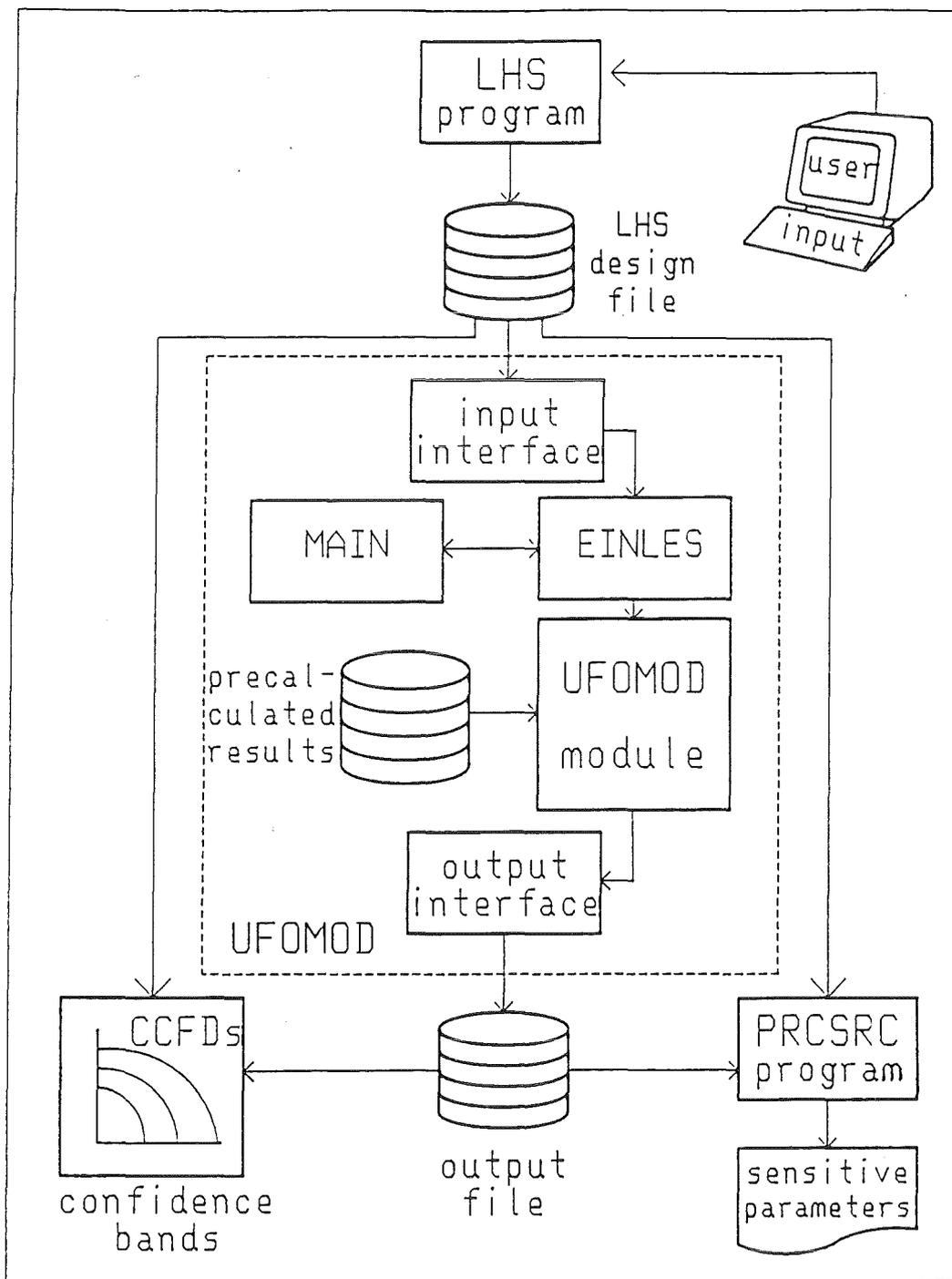


Figure 1. Scheme of UFOMOD - uncertainty and sensitivity analyses

For instance UFOMOD uncertainty analyses were done on a submodule basis and ended with a comprehensive overall uncertainty analysis. Therefore there was a need to compare the variation ranges of each consequence variable for each component analysis and the overall analysis. This was done by

- calculating e.g. the (5 %, 95 %) - limits of n (n = sample size) mean values or 99 % - quantiles (the horizontal 10^{-2} 'cutline' in the CCFD - (frequency, consequence) - diagram),
- presenting the corresponding sensitive parameters (from the submodule analyses and the final overall investigation) and their percentage contribution to the variation in the consequence variables.

Details to this kind of comparison and combination of results will not present here, but will be given in another report.

As a summarizing overview Figure 1 indicates in a schematic way the steps of uncertainty and sensitivity analyses done at KfK.

User defined characteristics (ranges, distributions, correlations) of uncertain model parameters serve as input to the Latin hypercube sampling program. The resulting design file of parameter values is needed to run UFOMOD via reading its input routine EINLES. When investigating one module, precalculated results obtained with the preceding module must be available; e.g. results from the atmospheric dispersion submodule are input to the countermeasures submodule. The output file contains the complete information to build CCFDs of consequence variables. A graphics program displays CCFDs and corresponding estimated confidence bounds. On the other hand the PRCSRC program is used to get the most sensitive parameters responsible for variations in consequences.

3. Uncertainty Analysis

The following Chapter 3.1 describes to some extent ranges, distributions and correlations of the model parameters, respectively.

Prior to the actual analysis performed with the program system UFOMOD it is necessary to define specific vectors of the uncertain model input parameters to be used in each run of UFOMOD. The selection of these sets of specific parameter values is done by a suitable *sampling scheme*. This is indicated in Chapter 3.2.. With *one* parameter set each run produces *one* complementary cumulative distribution function (CCFD). From all runs a set of curves results, which visualizes the variability of the CCFDs of consequences. Confidence bands can be derived together with sensitivity measures, which determine what causes this variability in consequences.

Important questions are, how to construct CCFD curves and confidence bands (see Chapter 3.3) how to calculate sensitivity measures and how many UFOMOD-runs are necessary to get reliable uncertainty and sensitivity results (see Chapter 3.4) ?

Uncertainty analysis methods may need much computer runs and time if there are a lot of model parameters and the accident consequence code is long-running. Therefore, one hand the designer of a sampling scheme should aim at a low number of runs, on the other hand the number of runs should be large enough to get stable and trustworthy results.

Mainly the uncertainty analysis codes from Sandia National Laboratories, Albuquerque NM (USA), are used (see [17] and [18]).

3.1 *Parameter Selection for the Submodule*

The countermeasures submodule of the program system UFOMOD models emergency actions assumed to be taken in the case of an accidental release of radionuclides. Depending on the type and amount of release, the dispersion conditions, the distance to the source, and time, the countermeasures may cover the whole range between minor important restrictions, almost without any impact on the average citizen, and disruption of normal living due to evacuation or relocation. Countermeasures are implemented with the aim of reducing either acute exposure during and shortly after the accident or continuing and long - term exposure due to deposited or incorporated radionuclides. In accident consequence assessment codes countermeasures are modelled in order to obtain realistic predictions of the consequences of an accidental release of radionuclides.

The results presented in this report require and use calculations from the atmospheric dispersion submodule of UFOMOD as precalculated input for the countermeasures submodule.

The following aspects of accident consequence assessments are investigated: The variability of the averaged³ individual acute doses (lung, bone marrow), individual risks (pulmonary, hematopoietic syndrome) at three distances: D1 (.875 km), D2 (4.9 km) and D3 (8.75 km) and the corresponding number of early fatalities.

In the early countermeasures module of UFOMOD, nine independent parameters were identified for consideration in this analysis. They are given in the following list and table together with their meaning and some rationale for the selection of ranges, distributions and correlation given in Table 1.

TINA (TINB)	initial delay of actions in area A (B) [h], where A is geometrically determined (keyhole - shaped) and area B is defined by an isodose line.
TDELA	delay time between end of release and end of sheltering period in area A [h]
PAUFA(i) (PAUFB(i))	<p>fraction of population with different behaviour during the sheltering period in area A (B)</p> <ul style="list-style-type: none"> • i = 1: spontaneous evacuation in cars at the start of the sheltering period. • i = 5: percentage of people who cannot be reached by the warning systems or stay outdoors intentionally. • i = 2,3,4: percentage of peoples sheltered in cellars and in buildings with low and high shielding factors, respectively. The condition $\sum_{i=1}^5 PAUFA(i) = 1$ led to the formulas given in Table 1.
GRWRTB	intervention dose level (IL) for emergency actions in area B
IEVA2	index of last outer radius of the keyhole-shaped area A
WGRNZA	angle of keyhole sector of area A (in degrees)
WSHIFT	azimuthal shift of the keyhole sector of area A against the wind direction of the first release phase (WSHIFT>0: rotation clockwise)

³ averaged over 144 weather sequences sampled from synoptic records of the two years 1982/83

No.	Parameter	Reference value	Distribution	Additional characteristics	Range of variation			Correlation of parameters
					w ₁ *)	w ₀ *)	w ₂ *)	
1	TINA	2	triangular		0.5	1	2.5	TINB 100% correlated to TINA
	TINB							
2	TDELA	0	triangular		0	2	4	
3	PAUFA(1)	0.3	triangular		0.333	1	1.666	$\sum_{i=1}^5 PAUFA(i) = 1$
4	PAUFA(5)	0.1	uniform		0		1	
	PAUFA(2)	$= [1 - (PAUFA(1) + PAUFA(5))]/2$						
	PAUFA(3)	$= [1 - (PAUFA(1) + PAUFA(5))]/4$						
	PAUFA(4)	$= [1 - (PAUFA(1) + PAUFA(5))]/4$						
	PAUFB(1)							PAUFB 100 % correlated to PAUFA
	PAUFB(2)							
	PAUFB(3)							
	PAUFB(4)							
	PAUFB(5)							
5	GRWRTB	0.5	uniform		0.2		1	
6	IEVA2	10	discrete	$p_{1,2,3} = \frac{1}{3}$	0.9	1.0	1.1	
7	WGRNZA	60	triangular		0.5	1.0	1.5	
8	WSHIFT	0	uniform		-15		+15	
9	TDRA	11.3	beta +)	$p=0.376$ $q=1.216$	0.35		3.10	
Note: *) $w_1 = w_{min}$ $w_0 = w_{50} = 50\%$ quantile $w_2 = w_{max}$ For TINA: w_0 means the peak value between w_1 and w_2 . In this case w_{50} is 1.28. +): TDRA means the 50th percentile of driving time in 10 km distance for the second population density class. All other driving time parameters are completely correlated to $TDRA \equiv TA(2,50)$ (10 km).								

Table 1. Reduced transformed parameter distribution table

Remark:

At the beginning of the uncertainty analyses studies for the countermeasure module of UFOMOD there was a list of twenty uncertain model parameters (12 TDRA(X,Y) - parameters and 8 other parameters). The first investigations showed only a small contribution of these driving time parameters on variations in consequences. Therefore, the list of parameters has been condensed to a parameter set of nine uncertain model parameters, i.e.:

12 TDRA(X,Y) - parameters have been condensed to *one* TDRA - parameter. For details see [9] .

□

3.2 *The sampling scheme*

There are various possible sampling strategies.

The *one-at-a-time-method* provides an estimate of the effect of a single parameter on consequences at selected fixed conditions of the other parameters. It is simple and can be thought as a sort of visual appreciation of the form of parameter-consequence dependence.

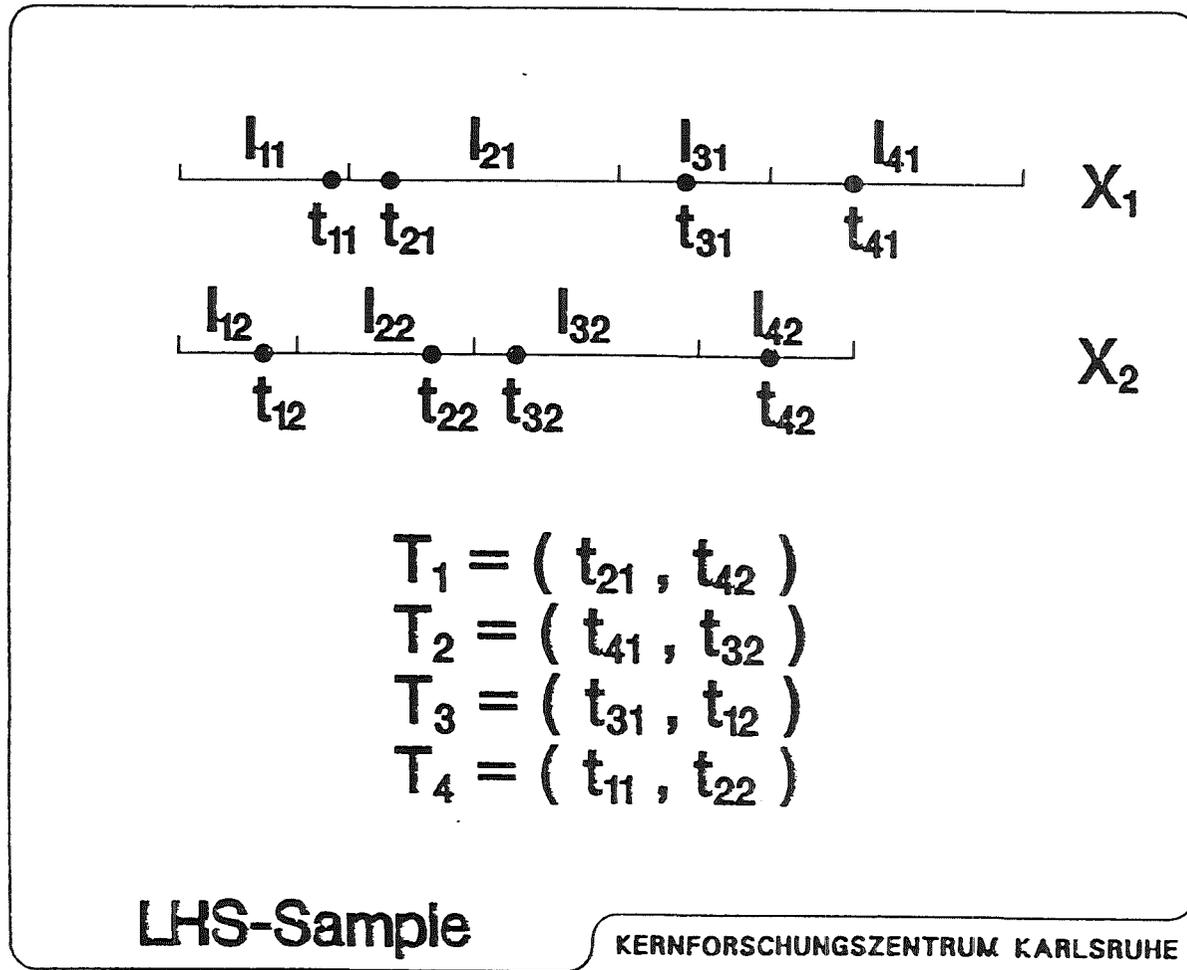
A *factorial design* utilizes two or more fixed values to represent each parameter under consideration. Unlike the one-at-a-time design the factorial design can detect and estimate interactions between uncertain model input parameters.

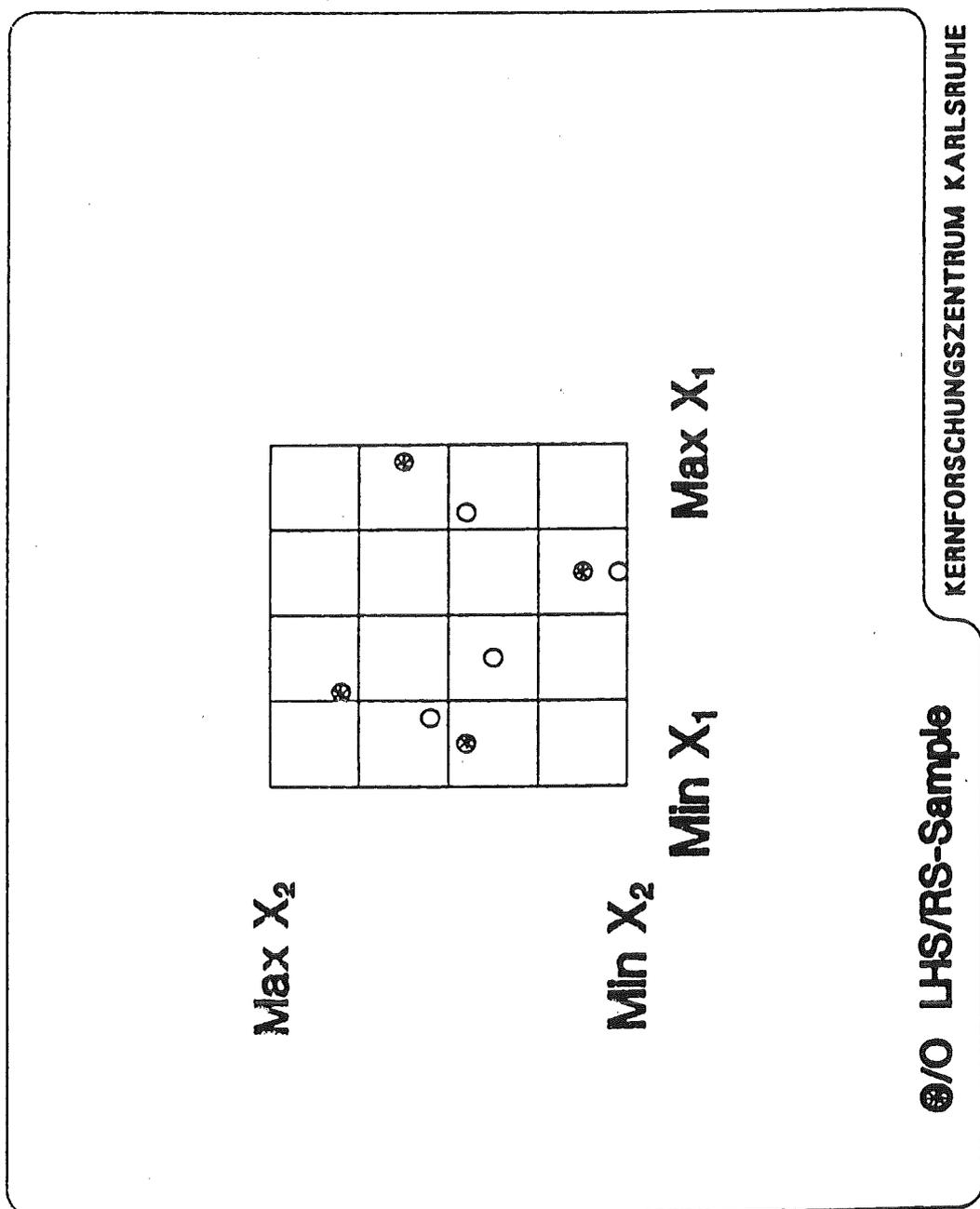
From the more sophisticated sampling strategies the Latin hypercube sampling (LHS) approach was selected. LHS is a modified random sampling with stratified samples and is found to have very good sampling characteristics when compared to other methods (see [16] and [22] (Vol. 3 K-5)).

The sampling procedure forces the value of each model parameter to be spread across its entire range. In random sampling it is possible by chance to choose only a portion of the range of model parameters, leaving out another part of the possible range that could greatly influence the consequence variables. The intent of LHS is to make more efficient use of computer runs than random sampling even for *smaller* sample sizes. For *large* sample sizes there is little difference between the two techniques.

A Latin hypercube sample of size n stratifies the range of each model parameter into " n " nonoverlapping intervals on the basis of equal probability. Randomly a value is selected from each of these intervals. Let X_i ($i=1,\dots,k$) be the model parameters. The n values 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 n k -tuples is formed.

This set of k -tuples is called a **Latin hypercube sample of size n** . As an example for ($n=2,k=4$) see the LHS - sample in Figure 2 and Figure 3.

Figure 2. LHS - sample construction for $n = 2, k = 4$ 



○/⊗ LHS/RS-Sample

Figure 3. Comparison Latin hypercube - and random - sample

There may exist "spurious" correlations between model parameter values within a Latin hypercube sample, due to the random pairing of the model parameter values in the generation of the sample. This is most likely when n is small in relation to k . Such correlations can be avoided by modifying the generation of the sample through use of a technique introduced by R.I. Iman and W.J. Conover [14]. This technique preserves the fundamental nature of LHS, but replaces the random pairing of model parameter values with a pairing that keeps all of the pairwise rank⁴ correlations among the k model parameters close to zero.

The Iman/Conover-technique can also be used to induce a desired rank correlation structure among the model parameters. The procedure is distribution free and allows exact marginal distributions to remain intact. This is used for the UFOMOD - LHS - design. For some mathematical details see [14], [8] and [10].

The parameter setup Figure 4 is corresponding to the requirements given in the SANDIA - LHS - user's guide [17]. For a complete reference and description of the LIIS - code the reader is urgently invited to make use of [17].

Keywords used in the parameter setup:

TITLE (optional)	This keyword can be followed with alphanumeric data to help describe the application of the sample. The information will be printed as an one-line header on each page of the output.
RANDOM SEED (required)	This keyword must be followed by an integer within the machine's range. This number is used as a starting point for the random number generator.
NREPS (optional)	This keyword can be used to generate multiple samples.
TRIANGULAR	This keyword requires an additional line of information containing three values a , b and c . The value b is the x-coordinate of the apex of the triangular distribution while a and c are the endpoints of the range.
UNIFORM	The second line of information provides, in order, the lower and upper endpoints of the interval that is to be sampled uniformly.
USER DISTRIBUTION	The setup for a three step discrete probability distribution is given with the same probability at the points .9, 1.0 and 1.1.

⁴ The rank order statistic for a random sample is any set of constants which indicate the order of observations. The actual magnitude of any observation is used only in the determination of its relative position in the sample array and is thereafter ignored in any analysis based on rank order statistics.

```

TITLE KFK LHS - DESIGN FOR UFOMOD (COUNTERMEASURES)
RANDOM SEED      87128436
NOBS  50
NREPS  1
TRIANGULAR                X(1) = TINA
.5    1  2.5
TRIANGULAR                X(2) = TDELA
0     2  4
TRIANGULAR                X(3) = PAUFA(1)
.333  1  1.666
UNIFORM                  X(4) = PAUFA(5)
0     1
UNIFORM                  X(5) = GRWRTB
.2    1
USER DISTRIBUTION        X(6) = IEVA2
3
.9    .333
1.0   .333
1.1   .333
TRIANGULAR                X(7) = WGRNZA
.5    1  1.5
UNIFORM                  X(8) = WSHIFT
-15  15
BETA                     X(9) = TDRA = TDRA(2,50)
.35  3.10    .3762  1.216
OUTPUT CORR HIST DATA

```

Figure 4. Parameter setup for generating a LHS - sample of size 50

Other examples of user defined distributions are possible. For details see [17].

BETA

The second line of information accompanying this keyword contains two values A and B specifying the endpoints of the distribution followed by two shape parameters p and q.

OUTPUT

This keyword is followed by one or more of three additional keywords. Their purpose is to control the amount of printer output.

- CORR

Both the raw and rank correlation matrices associated with the actual sample generated are printed.
- HIST

Histograms are generated for each variable in the sample based on the actual values of each variable in the sample.

- **DATA**

Each complete sample (50 observations on 9 variables) will be listed, followed by a complete listing of the ranks of each variable.

Up to now only those keywords have been listed in the keyword list which appear in the the parameter setup of the example Figure 4.

If the keyword **RANDOM SAMPLE** is used, the program produces a simple random sample instead of a Latin hypercube sample.

The use of the keyword **RANDOM PAIRING** allows the sampled values to be paired randomly instead of the restricted pairing technique of IMAN/CONOVER (see [14]).

The keyword **CORRELATION MATRIX** is used when it is desired to induce a rank correlation structure among the model parameters using the restricted pairing technique of IMAN/CONOVER (see [14]). If a correlation structure is *not* specified by the user, then the program computes a measure for detecting large pairwise correlations. This measure is called **variance inflation factor (VIF)** and is defined as the largest element on the diagonal in the inverse of the correlation matrix. As if VIF gets larger than 1, there may be some undesirably large pairwise correlations present. For details see the LHS manual [17].

The implemented list of possible distributions

- normal
- lognormal
- uniform
- loguniform
- triangular
- beta
- user defined distribution

can be extended easily.

Remarks concerning normal/lognormal distributions:

Following [17], normal and lognormal distributions are implemented as slightly truncated distributions. These distributions are concentrated on the range from A to B:

$$P(X_1 \leq A) = .001 \quad \text{and} \quad P(X_1 \geq B) = .001, \quad [4]$$

Thus

$$P(A \leq X_1 \leq B) = .998 \quad [5]$$

where $P(E)$ denotes the probability of event E . That is, A is defined as the .001 quantile and B is defined as the .999 quantile of the distribution of X_1 . The definitions of A and B imply that the mean of the normal (lognormal) truncated distribution is given by

$$\mu = (A + B)/2 \quad \text{or} \quad \mu = (\ln A + \ln B)/2 \quad [6]$$

and

$$\sigma^2 = [(B - \mu)/u_{.999}]^2 \quad \text{or} \quad \sigma^2 = [(\ln B - \mu)/u_{.999}]^2 \quad [7]$$

That is

$$\sigma^2 = [(B - A)/2 \cdot u_{.999}]^2 \quad \text{or} \quad \sigma^2 = [(\ln B - \ln A)/2 \cdot u_{.999}]^2 \quad [8]$$

$u_{.999}$ is the .999 quantile of the standardized normal random variable.

To summarize some facts about lognormal distributions:

A variable X has a lognormal distribution if $Y = \ln(X)$ has a $N(\mu, \sigma)$ distribution, where ($\mu \equiv \mu(y)$, $\sigma \equiv \sigma(y)$). The probability density function of X is given by

$$f(x) = [x \cdot \sigma \cdot \sqrt{2\pi}]^{-1} \cdot \exp\left\{-\frac{1}{2} \cdot \left[\left(\frac{\ln x - \mu}{\sigma}\right)^2\right]\right\} \quad [9]$$

Standardization of Y gives the new variable $U = (\ln x - \mu)/\sigma$. The lognormally distributed variable can be expressed as:

$$x \equiv x(u) = m \exp\{u \cdot \sigma\} \quad \text{with} \quad m = \exp\{\mu\} \quad [10]$$

Properties:

- $x_{median} \equiv x_{.50} = m$
- $x_\alpha \cdot x_{1-\alpha} = m^2$
- $\mu(x) = \exp\{\mu + (\sigma^2/2)\}$
- $\sigma^2(x) = \mu^2(x) \cdot (\exp\{\sigma^2\} - 1)$

□

If you want to use other truncation points the LHS - code has to be changed in the following way:

Example from LHS - Program (subroutine NORMAL):

```
C      IF IDT = 10  OR 11  THEN
C      A IS ASSUMED TO BE THE LOWER .100 QUANTILE OF THE NORMAL
C      DISTRIBUTION.
C      B IS ASSUMED TO BE THE UPPER .900 QUANTILE OF THE NORMAL
C      DISTRIBUTION.
C
      READ(8)A,B
      IF(IDT.EQ.11) THEN
          A=LOG(A)
          B=LOG(B)
      ENDIF
      PMU=(A+B)/2.
      IF (IDT.EQ.10.OR.IDT.EQ.11) THEN
          SIG=(B-PMU)/FINVNO(0.9)
          STRTPT=0.
          DO 10 I=1,N
              R=PROBIN*RAN( ISEED)+STRTPT
C              IF (R.GE.0.9)R=0.9
C              IF (R.LE.0.1)R=0.1
C
C          RR=CDF ( ALPHA)+(CDF ( 1.-ALPHA)-CDF ( ALPHA))*R
C
C          CDF (ALPHA)=0.1, CDF (1-ALPHA)=0.9, THEN RR=0.1+0.8*R
C
              RR=0.1+0.8*R
              X(LOC(I,J))=FINVNO(RR)*SIG+PMU
              IF (IDT.EQ.11)X(LOC(I,J))=EXP(X(LOC(I,J)))
              IF (IRS.EQ.0)STRTPT=STRTPT+PROBIN
10          CONTINUE
      ENDIF
```

Figure 5. Modified part of subroutine NORMAL in the LHS - code

```

//USERID   JOB (XXXX,YYY,ZZZZ),USRNAME,MSGCLASS=H,NOTIFY=USERID,
// REGION=2500K
//*MAIN LINES=5
//*
// EXEC F7CLG,PARM.C='XREF,LANGLVL(77) '
//C.SYSPRINT DD DUMMY
//* *****
//* LHS - FORTRAN SOURCE CODE
//*
//C.SYSIN DD DSN=USERID.NE89.FORT(LHSJ),DISP=SHR,LABEL=(,,IN)
//*
//* *****
//C.SYSUT2 DD UNIT=SYSDA,SPACE=(TRK,(100))
//* *****
//* LHS - DATA INPUT (see Figure 4)
//*
//G.SYSIN DD DSN=USERID.NE89.DATA(SG2LHS50),DISP=SHR
//*
//* *****
//* *****
//* LHS - DESIGN OUTPUT FILE
//*
//G.FT01F001 DD DSN=USERID.SG28850.UFOSAN,DISP=SHR,LABEL=(1,,OUT)
//*
//* *****
//G.FT02F001 DD UNIT=SYSDA,DCB=DCB.VBS
//G.FT03F001 DD UNIT=SYSDA,DCB=DCB.VBS
//G.FT04F001 DD UNIT=SYSDA,DCB=DCB.VBS
//G.FT07F001 DD UNIT=SYSDA,DCB=DCB.VBS
//G.FT08F001 DD UNIT=SYSDA,DCB=DCB.VBS
//G.FT09F001 DD UNIT=SYSDA,DCB=DCB.VBS
//

```

Figure 6. LHS - program job control for input corresponding to the previous parameter setup

TITLE KFK LHS - DESIGN FOR UFOMOD (COUNTERMEASURES)

RANDOM SEED = 87128436

NUMBER OF VARIABLES = 9

NUMBER OF OBSERVATIONS = 50

THE SAMPLE INPUT VECTORS WILL BE PRINTED ALONG WITH THEIR CORRESPONDING RANKS
HISTOGRAMS OF THE ACTUAL SAMPLE WILL BE PLOTTED FOR EACH INPUT VARIABLE
THE CORRELATION MATRICES (RAW DATA AND RANK CORRELATIONS) WILL BE PRINTED

TITLE KFK LHS - DESIGN FOR UFOMOD (COUNTERMEASURES)

VARIABLE	DISTRIBUTION	RANGE	LABEL
1	TRIANGULAR	WITH PARAMETERS BELOW	X(1) = TINA
		A= 0.500	
		B= 1.00	
		C= 2.50	
2	TRIANGULAR	WITH PARAMETERS BELOW	X(2) = TDELA
		A= 0.000E+00	
		B= 2.00	
		C= 4.00	
3	TRIANGULAR	WITH PARAMETERS BELOW	X(3) = PAUFA(1)
		A= 0.333	
		B= 1.00	
		C= 1.67	
4	UNIFORM	0.000E+00 TO 1.00	X(4) = PAUFA(5)
5	UNIFORM	0.200 TO 1.00	X(5) = GRWRTB
6	USER SUPPLIED DISTRIBUTION		X(6) = IEVA2
7	TRIANGULAR	WITH PARAMETERS BELOW	X(7) = WGRNZA
		A= 0.500	
		B= 1.00	
		C= 1.50	
8	UNIFORM	-15.0 TO 15.0	X(8) = WSHIFT
9	BETA	0.350 TO 3.10	X(9) = TDRA = TDRA(2,50)

WITH PARAMETERS P = 0.38 Q = 1.22
THIS CHOICE OF PARAMETERS GIVES A
POPULATION MEAN OF 1.00 AND A
POPULATION VARIANCE OF 0.526

Table 2. Echo of input parameters and input parameter distributions

Table 3. Example of actual Latin hypercube sample input vectors generated (Part 1)

TITLE KFK LHS - DESIGN FOR UFOMOD (COUNTERMEASURES)									PART 1
LATIN HYPERCUBE SAMPLE INPUT VECTORS									
NO.	X(1)	X(2)	X(3)	X(4)	X(5)	X(6)	X(7)	X(8)	X(9)
1	1.40	1.93	1.45	0.584	0.784	1.10	1.13	1.07	0.750
2	2.32	1.88	0.882	0.354	0.639	1.10	0.819	-4.84	0.350
3	1.47	1.56	0.633	0.875	0.483	1.10	1.35	-10.8	0.662
4	1.22	0.106	0.788	0.366	0.359	1.10	1.08	2.79	2.21
5	1.79	0.931	0.889	5.821E-02	0.562	1.00	0.976	9.22	0.436
6	1.13	3.35	1.36	9.678E-03	0.386	0.900	1.19	-1.47	0.637
7	1.51	2.81	1.49	0.937	0.669	1.10	1.29	-7.07	0.994
8	1.87	3.14	1.04	0.888	0.278	0.900	1.17	2.08	0.463
9	1.20	1.21	1.43	0.140	0.364	1.00	0.889	5.50	1.74
10	2.14	3.06	1.08	0.506	0.807	1.00	0.881	-3.05	0.388
11	1.75	2.08	1.12	0.482	0.500	0.900	0.914	8.50	0.356
12	0.882	1.86	1.21	0.978	0.686	0.900	1.00	4.21	2.63
13	0.937	1.65	1.19	0.529	0.257	1.00	0.669	-5.99	0.624
14	2.17	2.36	0.696	0.384	0.899	0.900	0.679	3.82	2.84
15	0.834	0.990	0.596	0.916	0.626	1.10	0.700	0.420	0.447
16	0.996	0.893	1.17	0.562	0.206	1.10	1.10	-8.74	1.27
17	2.07	2.66	0.814	0.444	0.334	1.00	1.05	7.92	0.572
18	1.06	3.67	1.16	0.332	0.531	1.10	0.981	11.1	0.420
19	1.29	2.60	0.977	0.781	0.607	0.900	1.23	-0.531	1.92
20	0.965	2.25	0.751	7.221E-02	0.661	1.10	1.17	12.8	0.863
21	1.70	1.38	0.484	0.422	0.433	0.900	1.25	-11.6	0.351
22	0.861	2.03	0.931	0.199	0.293	1.00	0.911	-11.1	1.10
23	0.803	1.72	0.624	0.847	0.994	1.00	1.01	-2.92	0.353
24	1.61	1.77	1.10	0.309	0.759	1.10	1.04	-14.6	1.47
25	1.32	2.88	0.677	9.220E-02	0.883	0.900	1.07	12.5	1.21

Table 4. Example of actual Latin hypercube sample input vectors generated (Part 2)

TITLE KFK LHS - DESIGN FOR UFOMOD (COUNTERMEASURES)									PART 2
LATIN HYPERCUBE SAMPLE INPUT VECTORS									
NO.	X(1)	X(2)	X(3)	X(4)	X(5)	X(6)	X(7)	X(8)	X(9)
26	1.24	2.50	0.722	0.663	0.457	1.00	1.42	-7.91	2.45
27	0.728	2.09	0.804	0.828	0.216	0.900	0.840	-10.1	0.370
28	0.634	2.26	0.769	0.237	0.772	1.10	0.950	13.7	0.359
29	1.54	2.31	1.10	0.767	0.851	1.10	0.512	-9.45	3.07
30	0.657	2.52	1.07	0.687	0.394	1.00	0.927	1.67	0.924
31	1.04	1.39	1.58	0.944	0.904	0.900	0.804	10.2	0.352
32	0.900	2.96	1.14	0.212	0.872	1.10	0.799	-4.48	0.363
33	1.02	3.46	0.845	0.103	0.722	1.10	0.778	-13.7	1.39
34	1.07	2.20	1.05	0.609	0.959	0.900	1.14	7.33	1.71
35	1.44	2.16	0.545	0.983	0.823	0.900	1.12	11.6	1.08
36	0.773	2.76	0.960	0.549	0.709	1.00	0.751	-12.1	0.510
37	1.67	1.11	1.00	0.814	0.303	0.900	0.726	14.1	0.817
38	1.85	1.83	0.857	0.729	0.569	0.900	0.999	-3.61	0.350
39	1.10	1.97	1.32	0.173	0.550	1.00	1.32	14.6	0.897
40	1.65	0.521	1.38	0.477	0.934	1.10	1.20	-6.03	0.394
41	1.26	2.44	1.28	0.271	0.508	1.00	1.11	9.79	0.551
42	2.00	2.72	1.23	0.637	0.248	0.900	0.606	-7.64	0.718
43	0.986	1.47	0.998	0.412	0.942	0.900	1.38	-14.3	0.479
44	1.92	1.64	1.25	0.700	0.741	1.00	0.847	-0.846	2.11
45	1.15	0.755	0.929	2.406E-02	0.587	1.00	1.02	-2.16	2.04
46	1.56	3.25	0.427	0.743	0.316	1.10	1.05	5.23	1.36
47	1.34	1.50	0.905	0.287	0.972	1.00	0.961	3.41	1.61
48	1.37	0.614	1.01	0.145	0.828	1.10	0.939	6.45	0.538
49	1.17	1.30	1.30	0.648	0.410	1.00	1.26	6.68	0.377
50	1.42	1.18	0.951	0.246	0.455	0.900	0.862	-12.7	0.404

Table 5. Echo of ranks of LHS sample values (Part 1)

TITLE KFK LHS - DESIGN FOR UFOMOD (COUNTERMEASURES)
RANKS OF LATIN HYPERCUBE SAMPLE INPUT VECTORS

RUN NO.	X(1)	X(2)	X(3)	X(4)	X(5)	X(6)	X(7)	X(8)	X(9)
1	30.	24.	48.	30.	37.	42.	37.	27.	27.
2	50.	23.	17.	18.	28.	42.	11.	17.	1.
3	33.	16.	6.	44.	18.	42.	48.	8.	25.
4	23.	1.	12.	19.	10.	42.	33.	30.	46.
5	42.	6.	18.	3.	23.	26.	23.	41.	15.
6	19.	48.	45.	1.	12.	9.	41.	23.	24.
7	34.	42.	49.	47.	30.	42.	46.	14.	32.
8	44.	46.	28.	45.	5.	9.	40.	29.	17.
9	22.	10.	47.	7.	11.	26.	16.	35.	42.
10	48.	45.	31.	26.	38.	26.	15.	20.	11.
11	41.	27.	34.	25.	19.	9.	18.	40.	6.
12	8.	22.	39.	49.	31.	9.	26.	33.	48.
13	10.	18.	38.	27.	4.	26.	3.	16.	23.
14	49.	34.	8.	20.	44.	9.	4.	32.	49.
15	6.	7.	4.	46.	27.	42.	5.	26.	16.
16	13.	5.	37.	29.	1.	42.	34.	11.	36.
17	47.	39.	14.	23.	9.	26.	31.	39.	22.
18	16.	50.	36.	17.	21.	42.	24.	44.	14.
19	26.	38.	24.	40.	26.	9.	43.	25.	43.
20	11.	31.	10.	4.	29.	42.	39.	47.	29.
21	40.	12.	2.	22.	15.	9.	44.	6.	3.
22	7.	26.	21.	10.	6.	26.	17.	7.	34.
23	5.	19.	5.	43.	50.	26.	27.	21.	5.
24	37.	20.	32.	16.	35.	42.	29.	1.	39.
25	27.	43.	7.	5.	43.	9.	32.	46.	35.

Table 6. Echo of ranks of LHS sample values (Part 2)

TITLE KFK LHS - DESIGN FOR UFOMOD (COUNTERMEASURES)
RANKS OF LATIN HYPERCUBE SAMPLE INPUT VECTORS

RUN NO.	X(1)	X(2)	X(3)	X(4)	X(5)	X(6)	X(7)	X(8)	X(9)
26	24.	36.	9.	34.	17.	26.	50.	12.	47.
27	3.	28.	13.	42.	2.	9.	12.	9.	9.
28	1.	32.	11.	12.	36.	42.	21.	48.	7.
29	35.	33.	33.	39.	41.	42.	1.	10.	50.
30	2.	37.	30.	35.	13.	26.	19.	28.	31.
31	15.	13.	50.	48.	45.	9.	10.	43.	4.
32	9.	44.	35.	11.	42.	42.	9.	18.	8.
33	14.	49.	15.	6.	33.	42.	8.	3.	38.
34	17.	30.	29.	31.	48.	9.	38.	38.	41.
35	32.	29.	3.	50.	39.	9.	36.	45.	33.
36	4.	41.	23.	28.	32.	26.	7.	5.	19.
37	39.	8.	26.	41.	7.	9.	6.	49.	28.
38	43.	21.	16.	37.	24.	9.	25.	19.	2.
39	18.	25.	44.	9.	22.	26.	47.	50.	30.
40	38.	2.	46.	24.	46.	42.	42.	15.	12.
41	25.	35.	42.	14.	20.	26.	35.	42.	21.
42	46.	40.	40.	32.	3.	9.	2.	13.	26.
43	12.	14.	25.	21.	47.	9.	49.	2.	18.
44	45.	17.	41.	36.	34.	26.	13.	24.	45.
45	20.	4.	20.	2.	25.	26.	28.	22.	44.
46	36.	47.	1.	38.	8.	42.	30.	34.	37.
47	28.	15.	19.	15.	49.	26.	22.	31.	40.
48	29.	3.	27.	8.	40.	42.	20.	36.	20.
49	21.	11.	43.	33.	14.	26.	45.	37.	10.
50	31.	9.	22.	13.	16.	9.	14.	4.	13.

Table 7. Echo of correlations among input values created by LHS for raw/rank data

TITLE KFK LHS - DESIGN FOR UFOMOD (COUNTERMEASURES)
 CORRELATIONS AMONG INPUT VARIABLES CREATED BY THE LATIN HYPERCUBE SAMPLE FOR RAW DATA

1	1.0000								
2	0.0275	1.0000							
3	-0.0397	-0.0224	1.0000						
4	0.0463	0.0246	-0.0284	1.0000					
5	-0.0188	-0.0110	0.0097	-0.0436	1.0000				
6	-0.1286	-0.0765	0.0107	-0.1892	0.0964	1.0000			
7	-0.0765	-0.0350	-0.0284	-0.0127	-0.0113	-0.0110	1.0000		
8	0.0022	0.0187	0.0471	-0.0844	0.0756	-0.1077	0.0626	1.0000	
9	0.0419	-0.0250	-0.0546	0.0538	0.1259	0.0079	-0.0763	-0.0385	1.0000
	1	2	3	4	5	6	7	8	9

VARIABLES

THE VARIANCE INFLATION FACTOR FOR THIS MATRIX IS 1.09

TITLE KFK LHS - DESIGN FOR UFOMOD (COUNTERMEASURES)
 CORRELATIONS AMONG INPUT VARIABLES CREATED BY THE LATIN HYPERCUBE SAMPLE FOR RANK DATA

1	1.0000								
2	0.0025	1.0000							
3	-0.0088	-0.0175	1.0000						
4	0.0572	0.0212	-0.0119	1.0000					
5	-0.0259	-0.0100	-0.0208	-0.0387	1.0000				
6	-0.1294	-0.0555	0.0134	-0.1916	0.0941	1.0000			
7	0.0211	-0.0195	-0.0108	0.0093	-0.0059	-0.0050	1.0000		
8	0.0194	0.0324	0.0438	-0.0805	0.0750	-0.1126	0.0832	1.0000	
9	0.0023	0.0672	0.0073	-0.0189	0.0105	0.0639	0.0703	0.0054	1.0000
	1	2	3	4	5	6	7	8	9

VARIABLES

THE VARIANCE INFLATION FACTOR FOR THIS MATRIX IS 1.09

Corresponding to the scheme given in Figure 1 the parameter sets from the LHS - design are used as input to a command procedure (CLIST - procedure). All work is done automatically by a so-called 'net job'. An UFOMOD run with a certain parameter set coming from the LHS - design starts if the predecessor run was completed successfully. The (x,y) - coordinates of the UFOMOD - CCFD curves are stored in the files 23, 24 and 34. Some hints to the contents of the command procedure are given in Figure 7 to Figure 9:

FILE 8	source term data
FILE 11	meteorological data
FILE 13	starting times for weather sequences
FILE 14 to 17	correction factors for cloudshine
FILE 40	nuclide data file
FILE 31	population data file
FILE 22	precalculated activity concentrations
FILE 41 to 43	dose conversion factors
FILE 23	(x,y) - coordinates for CCFDs (doses)
FILE 24	(x,y) - coordinates for CCFDs (risks)
FILE 34	(x,y) - coordinates for CCFDs (fatalities)
FILE 47	parameter sets from LHS - design (or parameter set for reference run, respectively)

```

PROC 2 START STOP LAST(51) NET1(YY) NET2(ZZ)
CONTROL NOFLUSH MSG NOLIST NOCONLIST
/*
/* ***** */
/* *
/* * CLIST TO START JOB'S *
/* * *
/* * IF THERE ARE MORE THAN 99 JOBS (135) USE : *
/* * SGM50RED 1 99 AND WHEN JOB USERID99 IS FINISHED : *
/* * SGM50RED 100 135 . (NET1 IS USERIDXX, NET2 IS USERIDZZ) *
/* * *
/* * TO USE MORE THAN 2 CALLS USE NET1(AB) NET1(GG) ... *
/* * THE "STOP" JOB ALWAYS IS ON HOLD. *
/* * ATTENTION: TO USE &ISOPAR TYPE &&ISOPAR *
/* * &END TYPE &&END *
/* * *
/* ***** */
/*
/* ERROR - HANDLING: INPUT ERROR
/*
IF &START > &STOP THEN +
    DO
        WRITE ERROR !!! ( START > STOP )
        GOTO FERTIG
    END
IF &STOP > &LAST THEN +
    DO
        WRITE ERROR !!! ( STOP > &LAST )
        GOTO FERTIG
    END
/*
SET COUNT = &START
IF &COUNT < 100 THEN +
    SET NET = &NET1
ELSE +
    SET NET = &NET2
/*
ANFANG: RETURN
/* ZAEHL MUST HAVE THREE DIGITS. IF NECESSARY INCLUDE LEADING ZERO.
IF &LENGTH(&COUNT) = 3 THEN SET ZAEHL = &STR(&COUNT)
IF &LENGTH(&COUNT) = 2 THEN SET ZAEHL = &STR(0&COUNT)
IF &LENGTH(&COUNT) = 1 THEN SET ZAEHL = &STR(00&COUNT)
SET SH1 = &SUBSTR(2:3,&ZAEHL)
/*
IF &COUNT = &LAST THEN SET ZAEHL = &STR(001)
SET HELP = &COUNT+1
IF &LENGTH(&HELP) = 3 THEN SET NR = &STR(&HELP)
IF &LENGTH(&HELP) = 2 THEN SET NR = &STR(0&HELP)
IF &LENGTH(&HELP) = 1 THEN SET NR = &STR(00&HELP)
SET SH2 = &SUBSTR(2:3,&NR)
/*

```

Figure 7. Command procedure to run UFOMOD with different parameter sets from LHS-design
(Part 1):
Partial echo from USERID.PROC.CLIST(SGM50RED)

```

WRITE
WRITE COUNT = &COUNT   ==>   ZAEHL = &ZAEHL   ==>   SH1 = &SH1
WRITE
SUBMIT * END(@@)
&STR(//USERID&SH1 JOB (XXXX,YYY,ZZZZ),USRNAME, )
IF &COUNT = &LAST | &COUNT = &LAST-1 | &COUNT = &STOP THEN +
&STR(// MSGCLASS=N,TIME=40,REGION=2048K,NOTIFY=USERID )
ELSE +
&STR(// MSGCLASS=N,TIME=40,REGION=2048K )
IF &COUNT = &START THEN +
&STR(/&STR(/*)NET ID=USERID&NET,RL=USERID&SH2 )
ELSE +
IF &COUNT = &STOP THEN +
&STR(/&STR(/*)NET ID=USERID&NET,HC=1 )
ELSE +
&STR(/&STR(/*)NET ID=USERID&NET,RL=USERID&SH2,HC=1 )
&STR(//* MAIN ORG=RM003 )
&STR(//* MAIN SYSTEM=M7890 )
&STR(// EXEC F7LG,PARM.G='FLIB(DFB=YES)') )
&STR(//L.SYSLIN DD DSN=USERID.OBJ.UFO(SGMRED),DISP=SHR )
&STR(//G.FT05F001 DD * )
&STR(&ZAEHL 47 )
&STR(// DD DISP=SHR,DSN=USERID.NE874INP.DATA(SGM) )
&STR(//G.FT08F001 DD DISP=SHR,DSN=USERID.UNFDATA.FK25FR1,LABEL=(,,IN) )
&STR(//G.FT11F001 DD DISP=SHR,DSN=USERID.DRSBWET.DATA,LABEL=(,,IN) )
&STR(//G.FT13F001 DD DISP=SHR,DSN=USERID.STRTZEIT.DATA,LABEL=(,,IN) )
&STR(//G.FT18F001 DD DUMMY )
&STR(//G.FT14F001 DD DISP=SHR,DSN=USERID.DRSB.GAMDAT(HOEHE10), )
&STR(// LABEL=(,,IN) )
&STR(//G.FT15F001 DD DISP=SHR,DSN=USERID.DRSB.GAMDAT(HOEHE50), )
&STR(// LABEL=(,,IN) )
&STR(//G.FT16F001 DD DISP=SHR,DSN=USERID.DRSB.GAMDAT(HOEHE100), )
&STR(// LABEL=(,,IN) )
&STR(//G.FT17F001 DD DISP=SHR,DSN=USERID.DRSB.GAMDAT(HOEHE200), )
&STR(// LABEL=(,,IN) )
&STR(//G.FT40F001 DD DISP=SHR,DSN=USERID.HEADER.DATA,LABEL=(,,IN) )
&STR(//G.FT20F001 DD UNIT=SYSDA,DCB=DCB.VBS )
&STR(//G.FT31F001 DD DISP=SHR,DSN=USERID.GUW.BEVNAH, )
&STR(// LABEL=(,,IN) )
&STR(//G.FT22F001 DD DSN=USERID.CONCEN.FK25FR1,DISP=SHR, )
&STR(// UNIT=SDG01,VOL=SER=INR003,LABEL=(,,IN), )
&STR(// DCB=(RECFM=VBS,BLKSIZE=13030) )
&STR(//G.FT25F001 DD UNIT=SYSDA,DCB=DCB.VBS,SPACE=(TRK,500) )
&STR(//G.FT26F001 DD UNIT=SYSDA,DCB=DCB.VBS )
&STR(//G.FT27F001 DD UNIT=SYSDA,DCB=DCB.VBS )
&STR(//G.FT28F001 DD UNIT=SYSDA,DCB=DCB.VBS )

```

Figure 8. Command procedure to run UFOMOD with different parameter sets from LHS-design (Part 2):
Partial echo from USERID.PROC.CLIST(SGM50RED)

```

&STR(//G.FT35F001 DD DUMMY )
&STR(//G.FT37F001 DD UNIT=SYSDA,DCB=DCB.VBS )
&STR(//G.FT41F001 DD DISP=SHR,DSN=USERID.DOSFAKEW.DATA, )
&STR(// ) )
DCB=(RECFM=F,BLKSIZE=23400) )
&STR(//G.FT42F001 DD DISP=SHR,DSN=USERID.DOSFAKEB.DATA, )
&STR(// ) )
DCB=(RECFM=F,BLKSIZE=23400) )
&STR(//G.FT43F001 DD DISP=SHR,DSN=USERID.DOSFAKIH.DATA, )
&STR(// ) )
DCB=(RECFM=F,BLKSIZE=23400) )
IF &COUNT = 1 THEN +
DO
&STR(//G.FT23F001 DD DISP=SHR,DSN=USERID.DOS8850.CCFD2 )
&STR(//G.FT24F001 DD DISP=SHR,DSN=USERID.RSK8850.CCFD2 )
&STR(//G.FT34F001 DD DISP=SHR,DSN=USERID.POP8850.CCFD2 )
END
ELSE +
DO
&STR(//G.FT23F001 DD DISP=(MOD,KEEP),DSN=USERID.DOS8850.CCFD2 )
&STR(//G.FT24F001 DD DISP=(MOD,KEEP),DSN=USERID.RSK8850.CCFD2 )
&STR(//G.FT34F001 DD DISP=(MOD,KEEP),DSN=USERID.POP8850.CCFD2 )
END
/* LAST RUN IS REFERENCE RUN !
IF &COUNT ^= &LAST THEN +
&STR(//G.FT47F001 DD DISP=SHR,DSN=USERID.SG28850.UFOSAN,LABEL=(,,IN) )
ELSE +
&STR(//G.FT47F001 DD DISP=SHR,DSN=USERID.SGM88RED.REF )
&STR(//* )
&STR(//* COUNTERMEASURE RUNS WITH NE88 FOR )
&STR(//* SANDIA - LHS - DESIGN )
&STR(//* )
&STR(//* OBJEKT.MODULE USERID.OBJ.UFO(SGMRED) PRODUCED BY )
&STR(//* USERID.UFOMOD.CNTL(ERZCON1) )
&STR(//* )
&STR(//* )
CONTROL MSG
@@
CONTROL NOMSG
IF &COUNT < &STOP THEN +
DO
/* WRITE NR = &COUNT
SET COUNT = &COUNT + 1
GOTO ANFANG
END
FERTIG: RETURN
EXIT

```

Figure 9. Command procedure to run UFOMOD with different parameter sets from LHS-design (Part 3):
Partial echo from USERID.PROC.CLIST(SGM50RED)

3.3 Estimation of confidence bounds

The next task is to run the accident consequence code with the sampled input parameter values from the LHS-design.

The following distinctions are necessary:

- There are stochastic variations e.g. in weather conditions or wind directions. Each run of UFOMOD therefore produces one frequency distribution (CCFD) of consequences.
- Due to lack of knowledge about the actual model parameter values there is an uncertainty in these results. This can quantitatively be expressed by confidence intervals of the frequency distribution of consequences.

CCFD curves are generated by considering the probability of equaling or exceeding each consequence level on the x-axis. To construct a CCFD keep in mind 144 weather sequences with different probabilities, say $PWET(L)$ ($L = 1, \dots, 144$), and 72 azimuthal sectors of 5° each, are considered. For each radius (distance) there exist 144×72 point values with the probability $PWET(L)/72$. The 144×72 consequence values are sorted into 90 classes (which correspond for instance to nine decades of consequence values on a logarithmic x-scale). Each class has its own probability of occurrence given by summing up the probabilities of the members of the class. Adding the probabilities of the classes stepwise from the right to the left will give the CCFD.

To get confidence curves for each consequence level so-called p-quantiles are calculated from the number n_0 of associated probability values at this consequence level x.

Example:

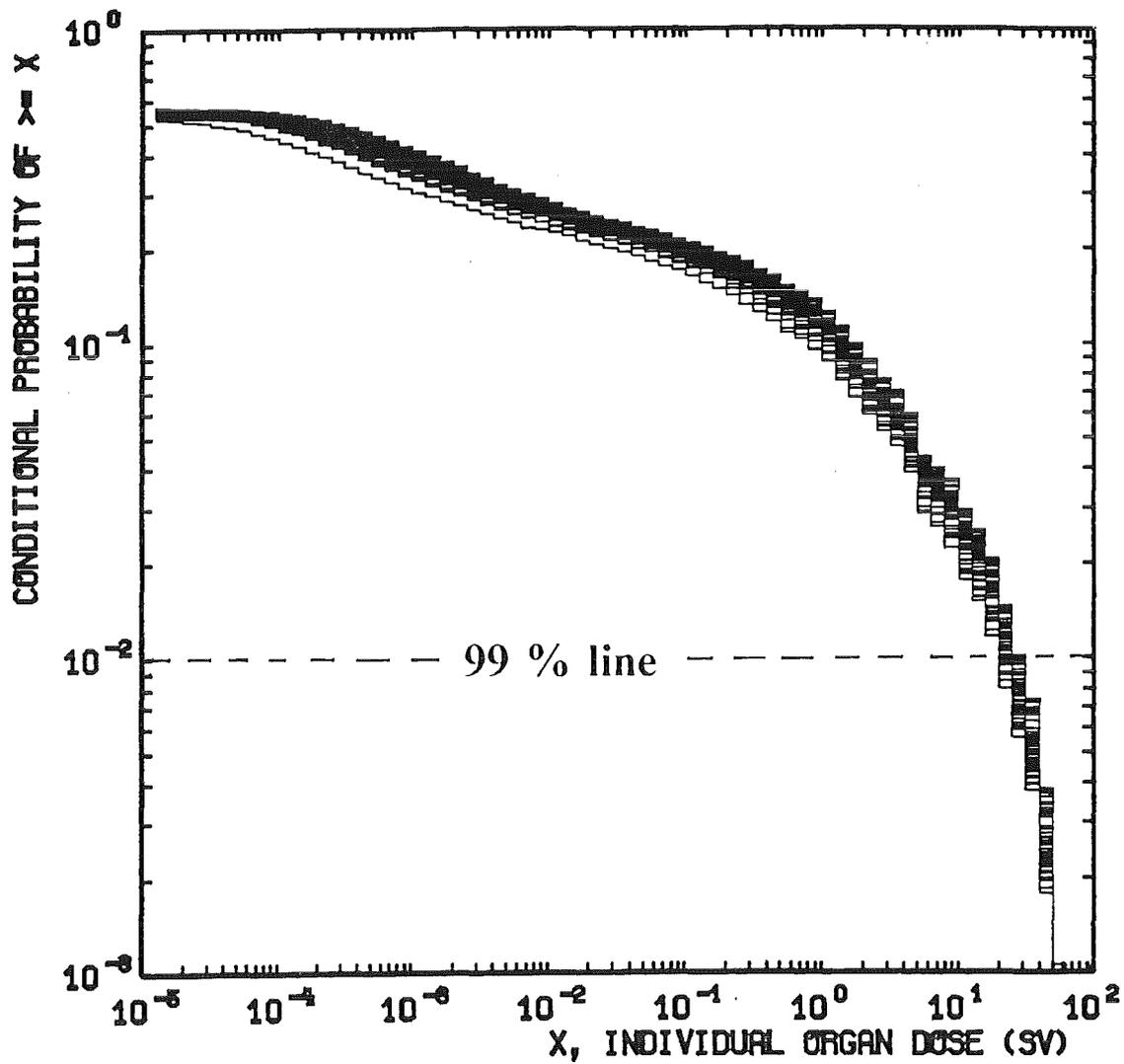
Suppose $n_0 = 60$ UFOMOD - runs, i.e. there are 60 CCFDs and - corresponding for each consequence level x - 60 probability points. To get a (p %) - confidence the following procedure has been adopted:

For each consequence level x find the (p %) - smallest probability value of n_0 ordered values. For all individual consequence levels these selected probability points are connected to obtain the estimated (p %) - confidence curve.

Particularly for the 5 % (95 %) - confidence curves connect the $p \times n_0$ -th numbers from the bottom in the ordered list of n_0 probability points, i.e. in our example connect the 3-rd and the 57-th values from the bottom, respectively. Mean and median curves can be created in a similar manner.

□

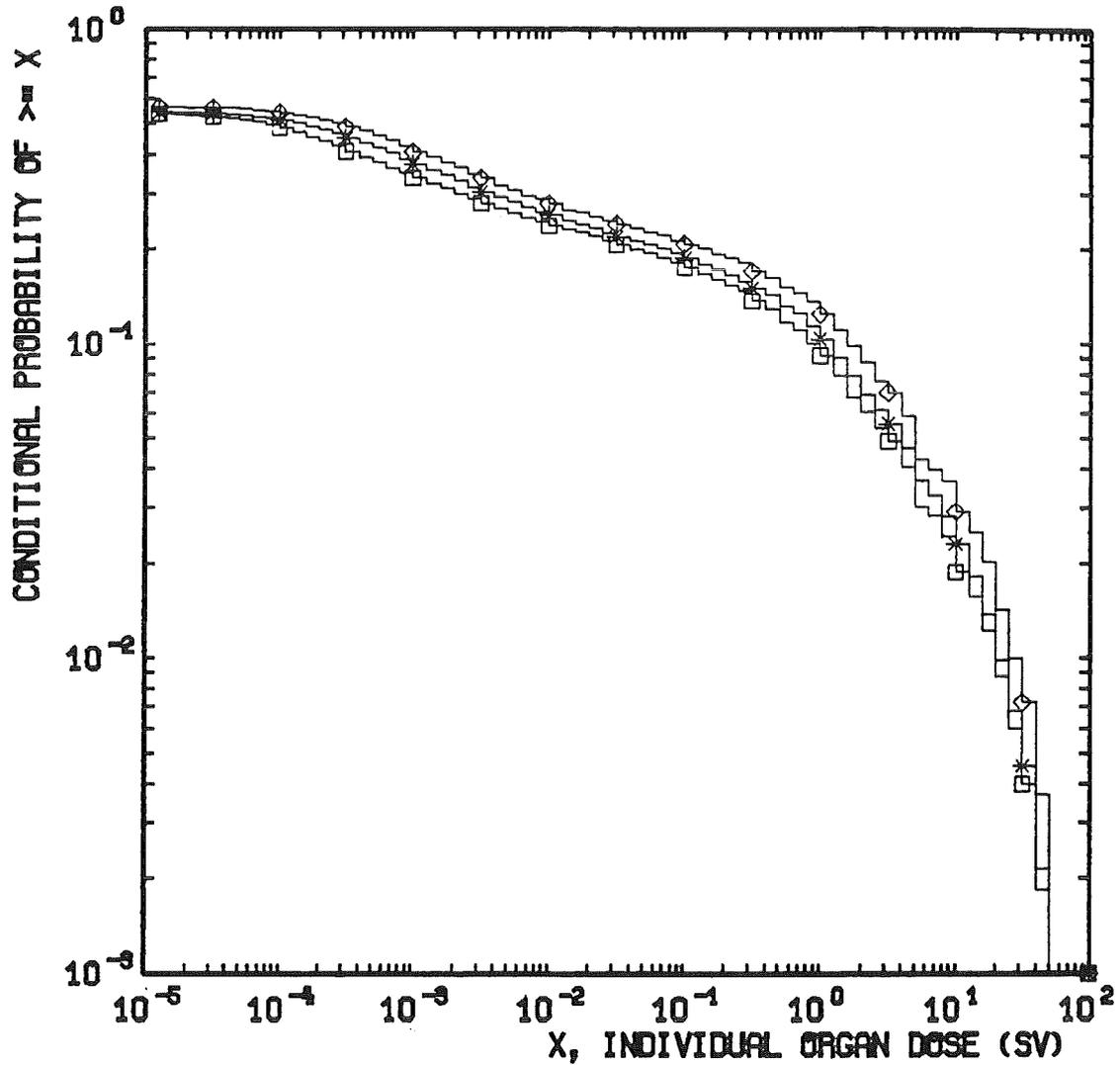
UFOMOD Uncertainty Analysis (1988)



Individual acute dose
Organ.....: lung
Distance: 0.875 km

Figure 10. Complementary cumulative frequency distributions (CCFDs) of acute individual lung dose values: Each CCFD (assuming release has occurred) corresponds to one of the 60 runs in a Latin hypercube sample of size 60.

UFOMOD Uncertainty Analysis (1988)



Individual acute dose
 Organ.....: Lung
 Distance: 0.875 km

* : Ref.-Curve
 □ : 5% -Curve
 ◆ : 95% -Curve

Figure 11. Reference CCFD of acute individual lung dose values: The empirical 5%-,95%-quantiles are given as estimated confidence bounds at discrete points of the x-axis.

It has been tested that different samples for $n=50$ (all driving time parameters, TDRA, are completely correlated) and for $n=60$ (TDRA parameters are partly correlated) do not change the 5%-95%-confidence bands.⁵ Figure 10 shows 60 estimated complementary cumulative frequency distributions for the acute individual dose values at the distance of .875 km. Figure 11 shows the corresponding estimated so-called *reference CCFD* (all uncertain input model parameters are at their point value (50%-quantile)) and the empirical 5%-95%-quantiles at each consequence level. The 5%-95%-'confidence curves' were generated by considering the probability of equaling or exceeding each consequence level appearing on the x-axis. For each consequence level the 5% and 95%-quantiles (or other values: mean, median etc.) were calculated from the 60 associated probability values. These probability estimates for individual consequence levels were then connected to obtain the empirical 5%-95%-confidence curves (see [1]).

So, the confidence bounds have to be interpreted as follows:

There is 90%-confidence that the conditional probability for the acute individual lung dose values, x , at 0.875 km distance, is

- below the ordinate value at x of the 95%-curve, and
- above the ordinate value at x of the 5%-curve.

The width of the CCFD-confidence band is an indicator of the sensitivity of model predictions with respect to variations in parameters, which are imprecisely known.

To present CCFDs the KfK - TRACEGS graphics system is used. It should be simple to modify the plot statements if different graphics systems are used (e.g.: DISSPLA). The construction of CCFDs and special CCFD-curves is done especially in the FORTRAN data set members GETID and COUNT. Some hints to the contents of the FORTRAN subroutines given in Figure 13:

GETID	subroutine reads the necessary general data and the pairs of (x,y) - coordinates and transforms to TRACEGS - (x,y) - arrays
ORDER	subroutine sorts one dimensional arrays in ascending order
COUNT	subroutine calculates special CCFD - curves: minimum, maximum, median, mean and p % values
DREMTY	subroutine calculates general figure frames without CCFDs
DRAWXY	subroutine calculates and draws CCFDs
DRTEXT	subroutine draws the text parts of the figures

⁵ In [16] is stated, that good results can be obtained even with $n = 4/3$ times the number of uncertain model parameters. For $n < k$ it seems appropriate to use the LHS - technique in a piecewise fashion on subsets of the k model parameters. For details see [14].

```

AT FIRST GENERAL INPUT FOR ALL FIGURES      <GETOD>      GLOBAL VALUES
-----
VALUE   NAME      MEANING
=====
FALSE  /TEST / PRODUCTION OF CONTROL OUTPUT
6      /NPRINT/ NR OF OUTPUT FILE (6 OR 12)
6      /NRPICS/ NUMBER OF FIGURES FOR THE COMPLETE JOB
'''    '''    '''    '''
----- NOW READ IN FOR LOG      X-AXIS  11 PARMS -----
15.0   /XLXE / LENGTH OF X - AXIS IN CM
1.E-5  /XMINXE/ STARTING POINT X - AXIS
1.E+2  /XMAXXE/ ENDPOINT X - AXIS
'''    '''    '''    '''
40     /ITXE / #{CHARACTERS) OF TEXTX (<0 - PARALLEL TO Y - AXIS)
        X, INDIVIDUAL ORGAN DOSE (SV)          ==> /TEXTX0/ CH#40 !
'''    '''    '''    '''
----- NOW READ IN FOR LOG      Y-AXIS  11 PARMS -----
15.0   /YLYE / LENGTH OF Y - AXIS IN CM
1.E-3  /YMINYE/ STARTING POINT Y - AXIS
1.E+0  /YMAXYE/ ENDPOINT Y - AXIS
'''    '''    '''    '''
-40    /ITYE / #{CHARACTERS) OF TEXTY (<0 - PARALLEL TO Y - AXIS)
        CONDITIONAL PROBABILITY OF >= X          /TEXTY0/
----- NOW AXIS PARMS FINISHED -----
.33    /HZS / HEIGHT OF SYMBOLS IN CM (* 0.857)
0      /INCS / TYPE(<0 SYMBOLS,0 LINES,1 BOTH,20 ALL 20 PAIRS)
60     /NRCURV/ #{CURVES) FOR EACH FIGURE
90     /NRVALS/ #{PAIRS) OF X,Y - VALUES
5      /LLOW / -- % LOWER CONFIDENCELIMIT
95     /LHIGH / -- % UPPER CONFIDENCELIMIT
D      /KONTYP/ TYP (D DOSIS, R RISK, P FATALITIES)
4      /KRING / DISTANCE RING (4,10,12 I.E.:.875 KM, 4.9 KM, 8.75 KM)
1      /NSYNDR/ (1 = LUNG, 2 = BONE MARROW)
D      /KONTYP/
10     /KRING /
1      /NSYNDR/
D      /KONTYP/
12     /KRING /
1      /NSYNDR/
D      /KONTYP/
4      /KRING /
2      /NSYNDR/
D      /KONTYP/
10     /KRING /
2      /NSYNDR/
D      /KONTYP/
12     /KRING /
2      /NSYNDR/
-----

```

Figure 12. Parameter setup for generating CCFD graphics (input):
Partial echo of USERID.GRAPH88C.IN(SGMDOS)

```

//USERID JOB (XXXX,YYY,ZZZZ),USRNAME,REGION=4096K,
// NOTIFY=USERID,MSGCLASS=H
//*MAIN LINES=15
// EXEC F7CLG,COMP=7NEU,
//      PARM.C='LANGVL(77),NOPRINT',
//      PLOT=GS7,
//      USER='TSOSYS.TRACEGS7'
//C.SYSIN DD DISP=SHR,DSN=USERID.GRAPH88C.FORT(MAIN)
//      DD DISP=SHR,DSN=USERID.GRAPH88C.FORT(GETOD)
//      DD DISP=SHR,DSN=USERID.GRAPH88C.FORT(REABAC)
//      DD DISP=SHR,DSN=USERID.GRAPH88C.FORT(GETID)
//      DD DISP=SHR,DSN=USERID.GRAPH88C.FORT(ORDER)
//      DD DISP=SHR,DSN=USERID.GRAPH88C.FORT(COUNT)
//      DD DISP=SHR,DSN=USERID.GRAPH88C.FORT(DREMTY)
//      DD DISP=SHR,DSN=USERID.GRAPH88C.FORT(DRAWXY)
//      DD DISP=SHR,DSN=USERID.GRAPH88C.FORT(DRTEXT)
//      DD DISP=SHR,DSN=USERID.GRAPH88C.FORT(DREND)
//L.SYSLIB DD
//      DD DISP=SHR,DSN=SYS2.CALCOMP
//L.SYSIN DD *
ORDER MAIN
//G.FT05F001 DD DISP=SHR,DSN=USERID.GRAPH88C.IN(SGMDOS)
//G.FT12F001 DD DISP=SHR,DSN=USERID.PR12.DATA
//G.FT30F001 DD DISP=SHR,DSN=USERID.GRAPH88C.IN(KOPF)
//G.FT32F001 DD DISP=SHR,DSN=USERID.GRAPH88C.IN(TYPD)
//G.FT33F001 DD DISP=SHR,DSN=USERID.GRAPH88C.IN(TYPR)
//G.FT34F001 DD DISP=SHR,DSN=USERID.GRAPH88C.IN(TYPP)
//G.FT35F001 DD DISP=SHR,DSN=USERID.GRAPH88C.IN(SYNDR1)
//G.FT36F001 DD DISP=SHR,DSN=USERID.GRAPH88C.IN(SYNDR2)
//G.FT37F001 DD DISP=SHR,DSN=USERID.GRAPH88C.IN(SYNDRD1)
//G.FT38F001 DD DISP=SHR,DSN=USERID.GRAPH88C.IN(SYNDRD2)
//G.FT40F001 DD DISP=SHR,DSN=USERID.GRAPH88C.IN(DISTO1)
//G.FT41F001 DD DISP=SHR,DSN=USERID.GRAPH88C.IN(DISTO2)
//G.FT42F001 DD DISP=SHR,DSN=USERID.GRAPH88C.IN(DISTO3)
//G.FT47F001 DD DISP=SHR,DSN=USERID.GRAPH88C.IN(DOSLHS1)
//G.FT48F001 DD DISP=SHR,DSN=USERID.GRAPH88C.IN(DOSLHS2)
//G.FT49F001 DD DISP=SHR,DSN=USERID.GRAPH88C.IN(OPTIL)
//G.FT57F001 DD DISP=SHR,DSN=USERID.GRAPH88C.IN(RSKLHS1)
//G.FT58F001 DD DISP=SHR,DSN=USERID.GRAPH88C.IN(RSKLHS2)
//G.FT67F001 DD DISP=SHR,DSN=USERID.GRAPH88C.IN(POPLHS1)
//G.FT68F001 DD DISP=SHR,DSN=USERID.GRAPH88C.IN(POPLHS2)
//G.FT17F001 DD DISP=SHR,DSN=USERID.XY.DATEN
//G.FT23F001 DD DISP=SHR,DSN=USERID.DOS8860.CCFD2,LABEL=(,,IN)
//G.COMM DD SYSOUT=#
//G.TRACEGS7 DD DISP=SHR,DSN=USERID.DOS8860.BILD
//

```

Figure 13. Job control for generating CCFD graphics (input):
Echo of USERID.GRAPH88C.CNTL(SGM8960)

Some hints to the contents of the input subroutines given in Figure 12:

FILE 23:	LHS - design file
FILE 30: KOPF	UFOMOD uncertainty analysis (1988)
FILE 32: TYPD	Individual acute dose
FILE 33: TYPR	Individual risk
FILE 34: TYPP	Early fatalities
FILE 35: SYNDR1	Health effect....: pulmonary syndrome
FILE 36: SYNDR2	Health effect....: hematopoetic syndrome
FILE 37: SYNDRD1	Organ.....: lung
FILE 38: SYNDRD2	Organ.....: bone marrow
FILE 40: DIST01	Distance.....: 0.875 km
FILE 41: DIST02	Distance.....: 4.9 km
FILE 42: DIST03	Distance.....: 8.75 km
FILE 47: DOSLHS1	Complementary cumulative frequency distributions (CCFDs) of acute individual organ doses (assuming release has occurred). Each CCFD corresponds to one of the 60 runs in a latin hypercube sample of size 60.
FILE 48: DOSLHS2	Reference CCFD of the acute individual organ doses (assuming release has occurred) and the empirical 5% -, 95% - quantiles respectively are given as estimated confidence bounds at discrete points of the x - axis.
FILE 57: RSKLHS1	CCFDs of individual risks
FILE 58: RSKLHS2	Reference CCFD of the individual risks
FILE 67: POPLHS1	CCFDs of early fatalities
FILE 68: POPLHS2	Reference CCFD of early fatalities
....DOS8860.BILD	Data set of stored CCFD - figures....

It is easy to change some FORTRAN - statements in subroutine DRTEXT, if the arrangement of the text lines and the corresponding contents has to be changed.

Remark:

The presentation of CCFD curves in this report is actually based on 60 UFOMOD runs and 20 underlying uncertain model parameters instead of 50 runs and only nine parameters. I.e. the twelve driving time parameters TDRA(X,Y) are not condensed to only *one* TDRA parameter, because we started with the complete parameter set at first. Later on we detected that this parameter condensation did neither affect the CCFD curves nor the corresponding sensitivity importance ranking. For details see [9].

□

3.4 Sensitivity analysis

Those uncertain input model parameters have to be identified which are important contributors to variations in consequences. Following [16], there are several methods for quantifying the relative importance of the uncertain model parameters to the output of the accident consequence model. Usually, each of the uncertain model parameters is ranked on the basis of its influence on the consequences. Some methods provide such an overall ranking while others (e.g. stepwise regression) are designed to select subsets consisting of only the most influential parameters.

- Rankings beyond the first few most important uncertain parameters usually have little or no meaning in an absolute ordering, since in many cases only a small number of the total number of uncertain parameters actually turns out to be significant. This will be explained later in more detail.
- Sensitivity analysis in conjunction with any form of sampling or design is easiest to carry out *if a regression model is fitted* between the model consequences and the model parameter values. Such a regression model is inherent in the calculation of correlation coefficients. But, regression techniques are influenced by extreme observations and nonlinearities. Therefore it seems to be appropriate to transform the data.

A method which

- is regression based,
- ranks either all uncertain model parameters or only those within a subset, and additionally
- avoids sophisticated transformations

is the ranking on the basis of *partial rank correlation coefficients*.

Now, *regression analyses* define the mathematical relationship between two (or more) variables, while *correlations* measure the strength of the relationship between two variables.

But do all correlation numbers indicate a significant relationship between variables, i.e. is there an actual relationship or only one by chance ('white noise')? Up to which level ('white noise'-level, critical value) the correlation numbers are treated as garbage?

The numerical values of correlation coefficients or partial (rank) correlations coefficients can be used for significance testing of the correlation, or with other words, for hypothesis testing to quantify the confidence in the correlation itself.

But to summarize the main results in advance:

To get **statistically stable results for sensitivity analyses** larger sample sizes than for confidence bounds calculations have to be chosen. The number of uncertain model parameters, which have a sensitivity measure value above the so-called 'white noise level' increase with sample size.

The **partial correlation coefficient (PCC)** is a measure that explains the linear relation between for instance a consequence variable and one or more uncertain model parameters with the possible linear effects of the remaining parameters removed. Following [12], when nonlinear relationships are involved, it is often more revealing to calculate PCCs between variable *ranks* than between the *actual values* for the variables. Such coefficients are known as **partial rank correlation coefficients (PRCCs)**. Specifically, the smallest value of each variable is assigned the rank 1, the largest value is assigned the rank n (n denotes the number of observations). The partial correlations are then calculated on these ranks.

The next step is to pick out the relevant sensitivity information of the bulk of hidden messages within the CCFDs.

There are various possible ways to condense the extensive data:

- Estimate fractiles, the estimated mean values etc. of the n CCFDs *at certain consequence levels*. There will be possibly divergent 'importance rankings' for different consequence values.
- Estimate fractiles, the estimated mean values etc. of the n CCFDs *at certain probability levels* (e.g.: 99 % values). There will be possibly divergent 'importance rankings' for different probability levels.
- Estimate *one* fractile, *one* estimated mean value etc. for each of the n consequence curves.

The second and third procedure is used for the UFOMOD - uncertainty and sensitivity analyses. To find the most important contributors to uncertainty in the consequences partial rank correlation coefficients (PRCCs) are used under assistance of the SANDIA PRCC-code (see [18]).

Importance ranking is done by taking *absolute* values of the PRCC values. The model parameter associated with the largest absolute PRCC value is called the **most important** one responsible for uncertainty in consequences and gets **importance rank 1**.

This differs from the definition of *ranks of sample values*, where the smallest values has rank 1, the next smallest has rank 2 and so on.

Example:

On the basis of 60 UFOMOD - runs with LHS, the most important uncertain parameters including their PRCC and *importance rank* for each consequence (e.g.: mean acute individual

lung dose values at the distance of .875 km) are identified. By statistical reasons (for mathematical details see Chap 3.4.2 and the corresponding example) a parameter is significant with confidence 95%, if the absolute value of the corresponding PRCC is greater than .31 (for $n=60$). The absolute value describes the strength of the input-output dependency, while the (+,-)-sign indicates increasing (decreasing) model consequences for increasing uncertain parameter values. The initial delay time of actions in area A, TINA, and the fraction of population, PAUFA(1), which evacuates spontaneously, are the most important sources of variation for the individual acute lung dose values with PRCC-values of .97 and -.84, respectively. Increasing TINA and decreasing PAUFA(1) lead to a strong increase of individual acute lung dose values (see Appendices).

□

In addition to evaluating the influence of each uncertain model parameter on the model consequences, the calculation of PCCs or PRCCs provide a good indicator of the 'fit of the analysis' to the model behaviour: the **coefficient of determination, R^2** , which is a measure of how well the linear regression model based on PCCs (or the corresponding standardized regression coefficients) can reproduce the actual consequence values. Or, in other words, it reflects the fraction of the variance in model consequences which can be explained by regression, i.e. it is possible to calculate the *percentage contribution* of each uncertain model parameter to variations in consequences. R^2 varies between 0 and 1 and is the square of the corresponding PCC. The closer R^2 is to unit, the better is the model performance.

3.4.1 Partial correlation coefficients

This paragraph follows some results presented in [12].

Sensitivity analysis in conjunction with Latin hypercube sampling is based on the construction of regression models. The observations

$$(X_{1i}, X_{2i}, \dots, X_{ki}, Y_i) \quad i = 1, \dots, n$$

are used to construct models of the form

$$Y_{est} = b_0 + \sum_q b_q Z_q$$

subject to the constraint that

$$\Sigma(Y - Y_{est})^2$$

be minimized. b_0, B_q are constants and each Z_q is a function of X_1, \dots, X_k .

An important property of least squares regression is that

$$\Sigma(Y - Y_m)^2 = \Sigma(Y - Y_{est})^2 + \Sigma(Y_{est} - Y_m)^2$$

where Y_m is the mean of the Y_i -values.

The R^2 - value (**coefficient of determination**) for a regression falls between 0 and 1 and is defined by

$$R^2 = \frac{\Sigma(Y_{est} - Y_m)^2}{\Sigma(Y - Y_m)^2}$$

The closeness of an R^2 - value to 1 provides an indication of how successful the regression model is in accounting for the variation in Y .

For a regression model of the form

$$Y_{est} = b_0 + b_1Z$$

with an R^2 - value of r^2 , the number $sign(b_1)|r|$ is called the correlation coefficient between Y and Z , where $sign(b_1) = 1$ if $b_1 \geq 1$, and $sign(b_1) = -1$ if $b_1 < 1$. This number provides a measure of linear relationship between these two variables. When more than one independent variable is under consideration, *partial correlation coefficients* are used to provide a measure of the linear relationships between Y and the individual independent variables. The *partial correlation coefficient* between Y and an individual variable Z_p is obtained from the use of a sequence of regression models. The following two regression models are constructed:

$$Y'_{est} = a_0 + \sum_{q \neq p} a_q Z_q \quad \text{and} \quad Z'_{est} = c_0 + \sum_{q \neq p} c_q Z_q .$$

Then, the results of the two preceding regressions are used to define the new variables $Y - Y'_{est}$ and $Z_p - Z'_p$. By definition, the **partial correlation coefficient** between Y and Z_p is the simple correlation coefficient between $Y - Y'_{est}$ and $Z_p - Z'_p$. Therefore, the partial correlation coefficient provides a measure of the linear relationship between Y and Z_p with the linear effects of the other variables removed.

Example:

Sometimes the apparent correlation between two variables may be due in part to the direct influence on both of the other variables: Y and X_1 are correlated, but are both influenced by a variable X_2 . The influence of X_2 on Y and X_1 must be removed. *Simple linear regression* of Y resp. X_1 on X_2 gives:

$$Y' = \beta_0 + \beta_1 X_2, \quad X'_1 = \gamma_0 + \gamma_1 X_2$$

Define new variables $(Y - Y')$ and $(X_1 - X'_1)$. The simple correlation (based on the Pearson product moment correlation) between the 'residuals' $(Y - Y')$ and $(X_1 - X'_1)$ is called the **partial correlation coefficient between Y and X₁, given X₂** (i.e., the linear influence of X₂ on both Y and X₁ removed), and is denoted by $r_{1Y.2}$:

$$r_{1Y.2} = \frac{r_{1Y} - r_{12}r_{Y2}}{\sqrt{(1 - r_{12}^2)(1 - r_{Y2}^2)}} \quad [11]$$

r_{1Y} , r_{12} , r_{Y2} are simple Pearson product moment correlations of the corresponding variables. For more details see [16], [12], [13], [18] and [28].

□

3.4.2 Significance tests

Following [6], the well-known Pearson product-moment correlation formula can be used to estimate Pearson's partial correlation coefficient. Spearman's rank correlation ρ has also been extended to measure partial rank correlation.

Partial correlation coefficients (PRCs) are correlation coefficients on conditional distributions. The distribution of the partial correlation coefficients depends on the multivariate distribution function of the underlying variables. Therefore PRCs may not be directly used as test statistics in nonparametric tests.

Starting from some well-known theorems, we may nevertheless do some approximative tests and analyses.

Step 1:

Find the distribution of the sampling correlation coefficient for random variables (X, Y) with bivariate normal distribution.

Theorem (Pitman's test): (see [19])

Let $u_i = (x_i, y_i)$ ($i=1, \dots, n$) be a random sample from a bivariate normal distribution with correlation r . Let r_s be the sample correlation coefficient (Pearson's product moment coefficient):

$$r_s = \frac{\sum_i (y_i - y_m)(x_i - x_m)}{\left[\sum_i (y_i - y_m)^2 \sum_i (x_i - x_m)^2 \right]^{\frac{1}{2}}} \quad [12]$$

Let $r = 0$ then

$$T_s = r_s \sqrt{\frac{(n-2)}{(1-r_s^2)}} \quad [13]$$

is distributed as Student's t with $(n-2)$ degrees of freedom.

□

Theorem: (see [20] or [23])

Let (z_1, \dots, z_k) be a random sample from a k -dimensional normal distribution and $r_{ij, u_1, \dots, u_p} = 0$ where r_{ij, u_1, \dots, u_p} is the partial correlation coefficient) of order p ($p = k-2$). u_1, \dots, u_p are $p = k-2$ numbers from $\{1, \dots, k\}$ which are different from i and j . That means the *partial* correlation between Z_i and Z_j is tested, say, while the indirect correlation due to Z_{u_1}, \dots, Z_{u_p} is eliminated. Let $r_{s; ij, u_1, \dots, u_p}$ be the sample partial correlation coefficient) of order p ($p = k-2$). Take n samples from the vector z , then

$$T_s = r_{s; ij, u_1, \dots, u_p} \sqrt{\frac{(n-2-p)}{(1-r_{s; ij, u_1, \dots, u_p}^2)}} \quad [14]$$

is distributed as Student's t with $(n-2-p)$ degrees of freedom.

□

Step 2:

Try to find adequate approximate formulas for non-normal situations.

Let $w_i = (u_i, v_i)$ ($i = 1, \dots, n$) be a random sample from a bivariate distribution with correlation r . Let r_s be the sample correlation coefficient. Transform the sample values (u_1, \dots, u_n) and (v_1, \dots, v_n) into their order statistics $(u_{(1)}, \dots, u_{(n)})$ and $(v_{(1)}, \dots, v_{(n)})$. Then do an *expected normal scores transformation*: Replace the order statistics of the (u, v) -variables by the expected value of the corresponding order statistics of standard normal variates (X, Y) . Then r_s transforms approximately to ψ_s :

$$r_s \sim \psi_s = \frac{\sum_i E(x_{(i)})E(y_{(i)})}{\sqrt{\sum_i E^2(x_{(i)}) \sum_i E^2(y_{(i)})}} \quad [15]$$

(This is clear from the hint that for a $N(0,1)$ -distributed variable X one has $\sum E(X_{(i)}) = 0$ because of $E(X_{(i)}) = -E(X_{(n-i+1)})$).

ψ_s can be used for an expected normal scores test of the hypothesis that U and V are uncorrelated.

[6] explains the role of the expected normal scores as well defined numbers which replace the unpleasant behaviour connected with using the order statistics from normal variables themselves. The procedure is based only on the ranks of the observations and is therefore a *rank test*.

Fisher and Yates (see [4]) suggested the analogue to Pitman's test using the exact normal scores instead of the the original data and applied the usual parametric procedures to these expected normal scores as a nonparametric procedure.

Step 3:

Give the significance test procedure.

The procedure is as follows:

The 'null' hypothesis reads: "No *partial* correlation exists between Y (the consequence variable) and X_i (one of the uncertain model parameters)", while the indirect influence due to the other model parameters is eliminated.

Then, for a sample of size n , the partial sample rank correlation, $\rho_{s;Y_i, u_1, \dots, u_p}$, between Y and X_i has to be calculated. ρ_s is then compared with the quantiles of the distribution of the test statistic. The comparison is made at a certain prescribed level of significance, α .

The 'null' hypothesis of *no* correlation is rejected, if the correlation value ρ_s leads to $|\rho_s| \geq T_{\alpha/2, n}$, the **critical value**, where $T_{\alpha/2, n}$ is a quantile of the test statistic's distribution.

$$T_{\alpha/2, n} \sim \frac{t_{\alpha/2, n-k}}{\sqrt{n-k + t_{\alpha/2, n-k}^2}} \quad [16]$$

$t_{\alpha/2, n-k}$ is the $(1 - \alpha/2)$ -quantile of the t-distribution with $n-k$ degrees of freedom (compare [15] or [21]). Eq. [16] is easily derived from Eq. [14].

Example:

For $n=50$ runs and $k=9$ uncertain input model parameters and $\alpha = 0.05$ (0.001) significance level, the partial rank correlation value (PRCC), ρ , is significant, if its absolute value is greater than 0.31 (0.49). This can be deduced from tables of the t-distribution (for instance: [15]), where the $(1 - \alpha/2)$ -quantile of the t-distribution with $n-k=41$ ($=50-9$) degrees of freedom is $t_{\alpha/2, n-k} = 2.0195(3.5442)$

□

Here some additional hints for motivation of the *coefficient of determination*, R^2 , are given.

The *total variation* of the consequence variable, Y , is defined as $\Sigma(Y - Y_m)^2$, i.e. the sum of squares of the deviation of values of Y from the mean Y_m .

$$\Sigma(Y - Y_m)^2 = \Sigma(Y - Y_{est})^2 + \Sigma(Y_{est} - Y_m)^2 \quad [17]$$

The first term on the right is called the *unexplained variation* while the second term is called the *explained variation* (by a regression model), so called because the deviations $(Y_{est} - Y_m)$ have a defined pattern while the deviations $(Y - Y_{est})$ behave in a random or unpredictable manner.

The ratio of explained variation to the total variation is called the *coefficient of determination*, R^2

$$R^2 = \frac{\Sigma(Y_{est} - Y_m)^2}{\Sigma(Y - Y_m)^2} \quad [18]$$

Remark:

In this report all R^2 - values R_t^2 , are normalized by R_s^2 .

$$R^2 = \left(\frac{R_s^2}{R_t^2} \right) \times 100, \quad [19]$$

where R_s^2 , R_t^2 are calculated by the SANDIA - PRCSRC-code (see [18]) and the R_t^2 - values are calculated with *all* (i.e. the complete set of) model parameters.

□

The calculation of the percentage contribution of each uncertain model parameter to the uncertainty in consequences is an easy but tedious task if a lot of uncertain model parameters and consequence variables have to be considered.

Hints:

Run the SANDIA - PRCSRC - code with the *complete* set of dependent variables (DEP VARS 1 14) and the *complete* set of independent variables (IND VARS 1 9), i.e. use the parameter setup identical to Figure 14. For each consequence variable the PRCSRC - program produces a R^2 - value. For instance it is $R^2 = 0.96$ with respect to the consequence variable DOSLUD1.

The next step is to find out the percentage contribution of a single input parameter (or a group of correlated parameters, if they exist) on the uncertainty in the consequence variable DOSLUD1.

```

TITLE AD-UFOMOD SENSITIVITY ANALYSIS ( COUNTERMEASURES )
NIV 9
NDV 14
NOBS 50
PRCC
STEPS 1 2 1
DEP VARS 1 2 3 4 5 6 7 8 9 10 11 12 13 14
IND VARS 1 2 3 4 5 6 7 8 9
FILE TYPE 5
TABLE CUTOFF .31
YLABEL DOSLUD1 DOSLUD2 DOSLUD3 DOSBMD1 DOSBMD2 DOSBMD3
      RSKLUD1 RSKLUD2 RSKLUD3 RSKBMD1 RSKBMD2 RSKBMD3
      POP(LU) POP(BM)
XLABEL TINA TDELA PAUFA(1) PAUFA(5) GRWRB IEVA2 WGRNZA WSHIFT TDRA

```

Figure 14. Parameter setup for running the PRCSRC - program:
Echo from USERID.NE89.DATA(SGPCCRED)

As an example input parameter no. 3, PAUFA(1), is taken. Then, make a change in row 8 of Figure 14 from (IND VARS 1 2 3 4 5 6 7 8 9) to (IND VARS 3) and run the PRCSRC - code with the modified parameter setup. The result is a value of $R^2 = 0.14$. By Eq. [19] this transforms to a percentage contribution of $R^2 = \left(\frac{0.14}{0.96} \right) \times 100 = 15\%$.

□

3.4.3 Examples of input and output for sensitivity calculations

To facilitate the understanding of the application of the sensitivity analysis code to UFOMOD (especially the user - supplied modification of the USRINP - subroutine) some details and echos of program parts are given.

```
//USERIDSL JOB (XXXX,YYY,ZZZZ),USRNAME,MSGCLASS=H,NOTIFY=USERID,
// REGION=2048K
//*MAIN LINES=10
//*MAIN ORG=RM011
//* *****
//*
//* VERSION OF PRCSRC WITHOUT PLOT - STATEMENTS AND -PLOT ROUTINES
//*
//* *****
//* // EXEC F7CLG,PARM.C='LANGLVL(77),OPT(0)',IMSL=SP
//*
//* // EXEC F7CLG,PARM.C='LANGLVL(77),DEBUG(SUBCHK,ARGCHK)'
// EXEC F7CLG,PARM.C='LANGLVL(77),NOPRINT'
//* //C.SYSPRINT DD SYSOUT=*
//C.SYSIN DD DSN=USERID.NE89.FORT(SGMPCC),DISP=SHR
//C.SYSUT2 DD UNIT=SYSDA,SPACE=(TRK,(100))
//G.SYSIN DD DSN=USERID.NE89.DATA(SGPCCRED),DISP=SHR
//*
//G.FT23F001 DD DSN=USERID.DOS8850.CCFD2,DISP=SHR,LABEL=(,,IN)
//G.FT24F001 DD DSN=USERID.RSK8850.CCFD2,DISP=SHR,LABEL=(,,IN)
//G.FT34F001 DD DSN=USERID.POP8850.CCFD2,DISP=SHR,LABEL=(,,IN)
//G.FT51F001 DD DSN=USERID.SG28850.UFOSAN,DISP=SHR,LABEL=(,,IN)
/*
```

Figure 15. PRCSRC - program job control for input to the previous parameter setup:
Echo from USERID.NE89.CNTL(SGMPCC)

The parameter setup Figure 14 is corresponding to the requirements given in the SANDIA - PRCSRC - user's guide [18]. For a complete reference and description of the PRCSRC - code the reader is urgently invited to look into [18].

Keywords used in the parameter setup:

TITLE (optional)

This keyword can be followed with alphanumeric data to help describe the application. The information will be printed as an one-line header on each page of the output.

NIV (required)	This keyword must be followed by a positive integer that specifies the number of independent variables (model input parameters) on the input file.
NDV (required)	This keyword must be followed by a positive integer that specifies the number of dependent variables (model outputs, consequence variables) on the input file.
NOBS (required)	This keyword must be followed by a positive integer that specifies the number of observations on the input file.
STEPS (optional)	This keyword must be followed by k ordered triples that specify the interval between successive readings of a particular dependent variable. The ordered triple means that reading were made on each dependent variable from step 1 to step 2 in increments of size 1.
PRCC (optional)	The partial correlation coefficients are computed on the ranks of the original observations when this keyword is used. This keyword can be used in conjunction with the keyword SRRC (standardized rank regression coefficients) in which both the PRCCs and SRRCs are computed and appear jointly in the output generated by the program. This keyword cannot be used in conjunction with the keywords PCC (partial correlation coefficient) and SRC (standardized regression coefficients) on <i>original</i> observations.
FILE TYPE (required)	This keyword must be followed by a positive integer that specifies one five file types for the input of the independent and dependent variables. We use FILE TYPE 5 only, i.e.: The user must supply coding to read input into arrays X and Y that are dimensioned as follows: X(NOBS, NIV) and Y(NOBS, NDV, NSTEPS) where NOBS, NIV and NDV have been defined previously and NSTEPS is the number of steps as ascertained from the keyword STEPS.
IND VARS (optional)	This keyword must be followed by a subset of the positive integers 1,2, ..., NIV that serves to indentify which of the independent variables are to be included in the analysis. If this keyword is omitted, all NIV independent variables are included in the analysis.
DEP VARS (optional)	This keyword must be followed by a subset of the positive integers 1,2, ..., NDV that serves to indentify which of the dependent variables are to be included in the analysis. If this keyword is omitted, all NDV independent variables are included in the analysis.
XLABEL (optional)	This keyword must be followed by identification labels for the NIV independent variables included in the analysis. If this

keyword is omitted, the generic labels X1, X2, ..., XNIV are used.

YLABEL (optional)

This keyword must be followed by identification labels for the NIV dependent variables included in the analysis. If this keyword is omitted, the generic labels Y1, Y2, ..., YNDV are used.

TABLE CUTOFF (optional)

This keyword must be followed by a real number p , $0 \leq p \leq 1$, which is activated, when the keyword STEPS indicates more than one step. When more than one step is indicated under the PRCC (or PCC) option, a summary table is automatically generated that shows the largest partial correlation for each independent variable - dependent variable combination over all steps, provided the the absolute value of the partial correlation is $\geq p$. Otherwise a blank entry appears for the combination. Similar statements hold for the options SRRC (or SRC). In the case of the pair PRCC and SRRC (or PCC and SRC) the table cutoff applies to the PRCCs (or PCCs).

In the following statements the tasks of the subroutine USRINP (see Figure 16 to Figure 20 are shortly described:

- IMODST=1 and DO - Loop no. 300 and 3001 serve to transform the CCFD - values into y - arrays. The calculation of PRCC - values can be done at predefined CCFD - steps k (i.e. for predefined consequence values).
- IMODST=2 and DO - loop no. 400 and 4001 serve to transform the CCFD - values into y - arrays. DO - Loop 501 calculates the weighted mean of y - values for each consequence variable.
- DO - loop no. 550 stores these mean values in two identical y - arrays. These two identical y - arrays and the x - array (the LHS - design file) are activated by (STEPS 1 2 1) (see row 6 in Figure 14). By this simple trick the summary table of PRCC values is activated.⁶
- At the end the 5% - and 95% - largest values of the mean values (for each consequence variable) and corresponding factors and differences are calculated. This allows to compare the variation ranges of each consequence variable for each component - and overall - uncertainty analysis.

⁶ The original PRCSRC - code has been modified at KIK to present PRCCs *and* the corresponding importance ranks in the summary table.

```

SUBROUTINE USRINP(X,Y,XB,XE,DX,
1XZWICH,XMEAN,XHILF,Y05,Y95,FACTOR,DIFFER)
C*****SUBROUTINE USRINP IS PROVIDED BY THE USER TO INPUT DATA FILES
C*****OF INDEPENDENT AND DEPENDENT VARIABLES THAT ARE OF DIFFERENT
C*****FORMS THAN THOSE DESCRIBED IN THE USER MANUAL
C*****THE COMMON AND DIMENSION STATEMENTS ARE REQUIRED
COMMON /MAXDIM/LENC, LENTC, LLAB, MXNDV, MXNINT, MXNIV,
1      MXNOBS, MXNSTP, NXSTEP, IMODST
COMMON /PARAM/LLN, LPCC, LPRCC, LSRC, LSRR, LRAW, NDV, NIV,
1      NINT, NOBS, NPLOTS, NSDV, NSIV, NSIVP1, NSTEPS,
2      PC, TC, YMIN, YMAX
DIMENSION DX(MXNINT),
1      X(MXNOBS,MXNIV), XB(MXNINT), XE(MXNINT),
2      Y(MXNOBS,MXNDV,MXNSTP)
DIMENSION XMEAN(MXNOBS,MXNDV),XHILF(MXNOBS),Y05(MXNDV),Y95(MXNDV),
1      XZWICH(MXNOBS,MXNDV),FACTOR(MXNDV),DIFFER(MXNDV)
DIMENSION CCFD(15,90,2),CCFDR(15,90,2),PKF(50,2)
DIMENSION CCWT(90),CCWTR(90),CCWTP(50)
CHARACTER*7 CVAR
C*****
C*****PROCESS THE INPUT KEYWORD RECORDS
IMAX=15
INK =2
C*****
REWIND 23
REWIND 24
REWIND 34
REWIND 51
C*****READ IN THE NONTRANSFORMED (ORIGINAL) INDEPENDENT VARIABLES
DO 102 I=1,NOBS
C      III=I
READ(51,ERR=130) IV,(X(I,J),J=1,NIV)
C      WRITE(6,5000) III
C      WRITE(6,5001) (X(I,J),J=1,NIV)
102 CONTINUE
5000 FORMAT(14)
5001 FORMAT(8G12.4)
C*****
C*****
C
IF (IMODST.EQ.2) THEN
DO 5555 JR=1,MXNINT
XB(JR) = 1
XE(JR) = 1
DX(JR) = 1
5555 CONTINUE
ENDIF

```

Figure 16. Subroutine USRINP in the PRCSRC - code (Part 1):
Partial echo from USERID.NE89.FORT(SGMPCC)

```

C
C*****
C*****READ IN THE DEPENDENT VARIABLES
      DO 200      II=1,NOBS
C*****
C***** COUNTERMEASURES (DOSES) INPUT START *****
C***** (JULY 1989)
C*****
      READ(23)      KDAT,
      *              ((CCFD(1,NGK,NOG),NOG=1,2),NGK=1,90),I=2,IMAX,2),
      *              (CCWT(IN),IN=1,90)
C*****
C***** COUNTERMEASURES (DOSES) INPUT END *****
C*****
C***** COUNTERMEASURES (RISKS) INPUT START *****
C***** (JULY 1989)
C*****
      READ(24)      KDAT,
      *              ((CCFDR(1,NGK,NOG),NOG=1,2),NGK=1,90),I=2,IMAX,2),
      *              (CCWTR(IN),IN=1,90)
C*****
C***** COUNTERMEASURES (RISKS) INPUT END *****
C*****
C***** COUNTERMEASURES (HEALTH EFFECTS) INPUT START *****
C***** (JULY 1989)
C*****
      READ(34)      KDAT,
      *              ((PKF(NGK,NOG),NOG=1,2),NGK=1,50),
      *              (CCWTP(NGK),NGK=1,50)
C*****
C***** COUNTERMEASURES (HEALTH EFFECTS) INPUT END *****
C*****
C*****
      IF (IMODST.EQ.1) THEN
          IL=1
          KK=0
          IXB=XB(1)
          IXE=XE(1)
          IDX=DX(1)
          DO 300      K= IXB,IXE,IDX
          KK=KK+ IL
          NOG=1
                                Y(II, 1, KK)      = (CCFD(4,K,NOG))
                                Y(II, 2, KK)      = (CCFD(10,K,NOG))
                                Y(II, 3, KK)      = (CCFD(12,K,NOG))

```

Figure 17. Subroutine USRINP in the PRCSRC - code (Part 2):
 Partial echo from USERID.NE89.FORT(SGMPCC)

```

      NOG=2
      Y(11, 4, KK) = (CCFD(4, K, NOG))
      Y(11, 5, KK) = (CCFD(10, K, NOG))
      Y(11, 6, KK) = (CCFD(12, K, NOG))

      NOG=1
      Y(11, 7, KK) = (CCFDR(4, K, NOG))
      Y(11, 8, KK) = (CCFDR(10, K, NOG))
      Y(11, 9, KK) = (CCFDR(12, K, NOG))

      NOG=2
      Y(11, 10, KK) = (CCFDR(4, K, NOG))
      Y(11, 11, KK) = (CCFDR(10, K, NOG))
      Y(11, 12, KK) = (CCFDR(12, K, NOG))
300  CONTINUE
      ENDIF
      IF (IMODST.EQ.1) THEN
      MXE=50
      IL=1
      KK=0
      IXB=XB(1)
      IXE=XE(1)
      IXE=MXE
      IDX=DX(1)
      DO 3001      K= IXB, IXE, IDX
      KK=KK+ IL
      NOG=1
      Y(11, 13, KK) = (PKF(K, NOG))

      NOG=2
      Y(11, 14, KK) = (PKF(K, NOG))
3001  CONTINUE
      ENDIF

      IF (IMODST.EQ.2) THEN
CFI *****
CFI MEANS
CFI *****
CFI

      DO 400 K=1, NXSTEP
      NOG=1
      Y(11, 1, K) = (CCFD(4, K, NOG))
      Y(11, 2, K) = (CCFD(10, K, NOG))
      Y(11, 3, K) = (CCFD(12, K, NOG))

      NOG=2
      Y(11, 4, K) = (CCFD(4, K, NOG))
      Y(11, 5, K) = (CCFD(10, K, NOG))
      Y(11, 6, K) = (CCFD(12, K, NOG))

```

Figure 18. Subroutine USRINP in the PRCSRC - code (Part 3):
Partial echo from USERID.NE89.FORT(SGMPCC)

```

      NOG=1
              Y(11, 7,K)      = (CCFDR(4,K,NOG))
              Y(11, 8,K)      = (CCFDR(10,K,NOG))
              Y(11, 9,K)      = (CCFDR(12,K,NOG))
      NOG=2
              Y(11,10,K)     = (CCFDR(4,K,NOG))
              Y(11,11,K)     = (CCFDR(10,K,NOG))
              Y(11,12,K)     = (CCFDR(12,K,NOG))
400  CONTINUE

      MXSTEP=50

      DO 4001 K=1,MXSTEP
      NOG=1
              Y(11,13,K)     = (PKF(K,NOG))
      NOG=2
              Y(11,14,K)     = (PKF(K,NOG))
4001  CONTINUE
      ENDIF
200  CONTINUE
      IF(IMODST.EQ.2) THEN
      DO 401 N=1,NDV

          IF( N.GE.13.AND.N.LE.14 )
1      NXSTEP=MXSTEP

      DO 501 I1=1,NOBS
      YZWZ = 0.
      YZWZ = YZWZ + Y(I1,N,NXSTEP)
      NNK = NXSTEP + 1
      DO 402 KK=1,NXSTEP
      K = NNK - KK
      K1= K-1
      IF (K1.EQ.0.) GOTO 402
      IF( N.GE.1.AND.N.LE.6 )
1      YZWZ = YZWZ + ( Y(11,N,K1)- Y(11,N,K) ) *CCWT(K)
      IF( N.GE.7.AND.N.LE.12)
1      YZWZ = YZWZ + ( Y(11,N,K1)- Y(11,N,K) ) *CCWTR(K)
      IF(N.GE.13.AND.N.LE.14)
1      YZWZ = YZWZ + ( Y(11,N,K1)- Y(11,N,K) ) *CCWTP(K)
402  CONTINUE
      XMEAN(I1,N) = YZWZ
501  CONTINUE
401  CONTINUE
      L05=5
      H05=L05*NOBS/100.
      N05=H05
      L95=95

```

Figure 19. Subroutine USRINP in the PRCSRC - code (Part 4):
Partial echo from USERID.NE89.FORT(SGMPCC)

```

H95=L95*NOBS/100.
N95=H95
WRITE(6,*) 'N05 = ',N05,' ',
1      'N95 = ',N95
DO 500   N= 1,NDV
IF (N.EQ. 1) CVAR='DOSLUD1'
IF (N.EQ. 2) CVAR='DOSLUD2'
IF (N.EQ. 3) CVAR='DOSLUD3'
IF (N.EQ. 4) CVAR='DOSBMD1'
IF (N.EQ. 5) CVAR='DOSBMD2'
IF (N.EQ. 6) CVAR='DOSBMD3'
IF (N.EQ. 7) CVAR='RSK LUD1'
IF (N.EQ. 8) CVAR='RSK LUD2'
IF (N.EQ. 9) CVAR='RSK LUD3'
IF (N.EQ.10) CVAR='RSK BMD1'
IF (N.EQ.11) CVAR='RSK BMD2'
IF (N.EQ.12) CVAR='RSK BMD3'
IF (N.EQ.13) CVAR='POP(LU)'
IF (N.EQ.14) CVAR='POP(BM)'
      DO 5730   NI= 1,NOBS
5730     XHILF(NI) = 0.
      CONTINUE
DO 555     II= 1,NOBS
      Y(II, N, 1)   =   XMEAN(II,N)
      Y(II, N, 2)   =   XMEAN(II,N)
      XHILF(II)     =   XMEAN(II,N)
555     CONTINUE
      CALL ORDER(NOBS,XHILF)
      Y05(N)        =   XHILF(N05)
      IF(Y05(N).EQ.0) Y05(N)=-1.000
      Y95(N)        =   XHILF(N95)
      FACTOR(N)     =   Y95(N)/Y05(N)
      DIFFER(N)     =   Y95(N)-Y05(N)
      WRITE(6,8811,ERR=500) CVAR,Y05(N),Y95(N),FACTOR(N),DIFFER(N)
8811  FORMAT(A15,5X,' 5 % VALUE = ',1PE10.2,5X,
1      '95 % VALUE = ',1PE10.2,5X,
2      '   FACTOR = ',1PE10.2,5X,
3      'DIFFERENCE = ',1PE10.2,5X)
500   CONTINUE
      ENDIF
C
      REWIND 23
      REWIND 24
      REWIND 34
      REWIND 51
130   CONTINUE
      RETURN
      END

```

Figure 20. Subroutine USRINP in the PRCSRC - code (Part 5):
 Partial echo from USERID.NE89.FORT(SGMPCC)

```

DO 501 I1=1,NOBS
YZWZ = 0.
NNK = NXSTEP + 1
DO 402 KK=1,NXSTEP
K1= KK
K = KK
IF (K1.EQ.0.) GOTO 402
IF( N.GE.1.AND.N.LE.6 .AND. Y(I1,N,K1).GE.1E-2)
1 YZWZ = CCWT(K)
IF( N.GE.7.AND.N.LE.12 .AND. Y(I1,N,K1).GE.1E-2)
1 YZWZ = CCWTR(K)
IF( N.GE.13.AND.N.LE.14 .AND. Y(I1,N,K1).GE.1E-2)
1 YZWZ = CCWTP(K)
402 CONTINUE
XZWICH(I1,N) = YZWZ
501 CONTINUE

```

Figure 21. Necessary modifications for USRINP in the PRCSRC - code for 99% - quantile evaluation:

Partial echo from USERID.NE89.FORT(SGM99PCC)

As mentioned above, the sensitivity analysis may be based on mean values or p - quantiles.

For example, if the PRCC - values should be based on the 99% - quantiles the modified DO - loop no. 501 (see Figure 21) has to be used instead of the corresponding part in the original part of the USRINP - subroutine. Or in other words, DO - loop no. 501 calculates the intersection points of the horizontal 99% - line (i.e. the 10^{-2} -line) with the CCFDs in Figure 10.

The original output sensitivity tables Table 8 and Table 9 contain in the leading rows the table cutoff value 0.31 from Figure 14, which is identical to the 'critical value' in the significance tests of Chap. 3.3.2.. The first horizontal line in the table contains the dependent variables from Figure 14 and the first column gives the independent parameters from Figure 14. The PRCC - values are presented in combination with their corresponding 'importance rank'.

The modified sensitivity tables Table 10 and Table 11 contain some additional information in the leading rows with respect to the 'critical value'. Manually added to the PRCC - values and their corresponding ranks are the percentage contribution values to uncertainty.

Table 8. Echo of original output sensitivity table (Part 1):
corresponding to Figure 14 and Figure 15

UFOMOD SENSITIVITY ANALYSIS (COUNTERMEASURES AUGUST '88)

PAGE 1

TABLE ENTRIES REPRESENT THE VALUE OF THE PARTIAL RANK CORREL. COEFFICIENT FOR EACH COMBINATION OF SELECTED INDEPENDENT VARIABLE AND SELECTED DEPENDENT VARIABLE, PROVIDED THAT THE ABSOLUTE VALUE OF THIS COEFFICIENT IS GREATER THAN 0.310

	DOSLUD1	DOSLUD2	DOSLUD3	DOSBMD1	DOSBMD2	DOSBMD3	RSK LUD1	RSK LUD2	RSK LUD3	RSK BMD1
TINA	.97(1)	.91(1)	.57(3)	.98(1)	.75(1)	.67(2)	.96(1)			.86(2)
TDELA		.40(6)	.53(4)							.65(4)
PAUFA(1)	-.87(2)	-.88(2)	-.87(2)	-.73(4)	-.49(5)	-.63(3)	-.87(2)			-.45(5)
PAUFA(5)	.56(4)	.64(3)		.86(2)	.62(4)	.54(4)	.68(3)			.98(1)
GRWRTB		.58(4)	.96(1)		.69(2)	.99(1)				
IEVA2		-.42(5)		.39(5)	-.64(3)		.35(5)			
WGRNZA	-.31(5)	-.33(8)					-.32(6)			-.41(6)
WSHIFT										
TDRA	.58(3)	.39(7)	.42(5)	.80(3)	.41(6)	.54(5)	.56(4)			.74(3)

UFOMOD SENSITIVITY ANALYSIS (COUNTERMEASURES AUGUST '88)

TABLE ENTRIES REPRESENT THE VALUE OF THE PARTIAL RANK CORREL. COEFFICIENT FOR EACH COMBINATION OF SELECTED INDEPENDENT VARIABLE AND SELECTED DEPENDENT VARIABLE, PROVIDED THAT THE ABSOLUTE VALUE OF THIS COEFFICIENT IS GREATER THAN 0.310

	RSKBMD2	RSKBMD3	POP(LU)	POP(BM)
TINA			.96(1)	.92(2)
TDELA				.68(3)
PAUFA(1)			-.89(2)	-.63(5)
PAUFA(5)			.77(3)	.98(1)
GRWRTB				
IEVA2			.42(5)	
WGRNZA			-.41(6)	-.31(7)
WSHIFT			-.32(7)	-.33(6)
TDRA			.61(4)	.68(4)

Table 9. Echo of original output sensitivity table (Part 2):
corresponding to Figure 14 and Figure 15

Table 10. Echo of modified output sensitivity table (Part 1):
corresponding to [9]

UFOMOD SENSITIVITY ANALYSIS (LHS-DESIGN)

COUNTERMEASURES

PART 1 OF 2

TABLE ENTRIES REPRESENT THE VALUE OF THE PARTIAL RANK CORRELATION COEFFICIENT (AND ITS RANK) FOR EACH COMBINATION OF SELECTED INDEPENDENT AND SELECTED DEPENDENT VARIABLE, PROVIDED THAT THE ABSOLUTE VALUE OF THIS COEFFICIENT IS GREATER THAN $T(\text{ALPHA}) = 0.31$ (50 RUNS, 9 PARAMETERS) FOR ALPHA = 0.05 SIGNIFICANCE LEVEL (E.G. THE CRITICAL VALUE IS $T(\text{ALPHA}) = 0.49$ (50 RUNS, 9 PARAMETERS) FOR ALPHA = 0.001 SIGNIFICANCE LEVEL)

50C, (C) MEANS: THE TDRA (I.E. TA) PARAMETERS ARE COMPLETELY (C) CORRELATED

THE PERCENTAGE CONTRIBUTIONS TO UNCERTAINTY ARE GIVEN FOR EACH INDEPENDENT PARAMETER

#RUNS	DOSLUD1		DOSLUD2		DOSLUD3		DOSBMD1		DOSBMD2		DOSBMD3	
	50C	(%)										
TINA	.97	(1) 81	.91	(1) 50	.57	(3) 2	.98	(1) 78	.75	(1) 37	.67	(2) 1
TDELA			.40	(6)	.53	(4)		1				
PAUFA(1)	-.87	(2) 15	-.88	(2) 33	-.87	(2) 21	-.73	(4) 4	-.49	(5) 9	-.63	(3) 1
PAUFA(5)	.56	(4) 3	.64	(3) 11			.86	(2) 12	.62	(4) 22	.54	(4)
GRWRB			.58	(4) 3	.96	(1) 73			.69	(2) 27	.99	(1) 96
IEVA2			-.42	(5) 7		1	.39	(5)	-.64	(3) 23		
WGRNZA	.31	(5)	-.33	(8) 1								
WSHIFT								1				
TDRA	.58	(3) 2	.39	(7) 1	.42	(5) 2	.80	(3) 6	.41	(6) 4	.56	(4) 1

Table 11. Echo of modified output sensitivity table (Part 2):
corresponding to [9]

UFOMOD SENSITIVITY ANALYSIS (LHS-DESIGN)		COUNTERMEASURES		PART 2 OF 2				
<p>TABLE ENTRIES REPRESENT THE VALUE OF THE PARTIAL RANK CORRELATION COEFFICIENT (AND ITS RANK) FOR EACH COMBINATION OF SELECTED INDEPENDENT AND SELECTED DEPENDENT VARIABLE, PROVIDED THAT THE ABSOLUTE VALUE OF THIS COEFFICIENT IS GREATER THAN $T(\text{ALPHA}) = 0.31$ (50 RUNS, 9 PARAMETERS) FOR ALPHA = 0.05 SIGNIFICANCE LEVEL (E.G. THE CRITICAL VALUE IS $T(\text{ALPHA}) = 0.49$ (50 RUNS, 9 PARAMETERS) FOR ALPHA = 0.001 SIGNIFICANCE LEVEL)</p> <p>50C, (C) MEANS: THE TDRA (I.E. TA) PARAMETERS ARE COMPLETELY (C) CORRELATED</p> <p>THE PERCENTAGE CONTRIBUTIONS TO UNCERTAINTY ARE GIVEN FOR EACH INDEPENDENT PARAMETER</p>								
#RUNS	RSKLU1		RSKBMD1		POP(LU)		POP(BM)	
	50C	(%)	50C	(%)	50C	(%)	50C	(%)
TINA	.96(1)	72	.86(2)	14	.96(1)	68	.92(2)	20
TDELA			.65(4)	4			.68(3)	4
PAUFA(1)	-.87(2)	19	-.45(5)	1	-.89(2)	20	-.63(5)	2
PAUFA(5)	.68(3)	7	.98(1)	80	.77(3)	9	.98(1)	76
GRWRTB								
IEVA2	.35(5)			2	.42(5)			3
WGRNZA	-.32(6)		-.41(6)		-.41(6)		-.31(7)	
WSHIFT		1		2	-.32(7)	1	-.33(6)	2
TDRA	.56(4)	2	.74(3)	4	.61(4)	3	.68(4)	2

4. Summary

The procedures presented in this user guide shall serve as a guidance on applications of uncertainty analysis methods and computer codes to accident consequence assessment codes, such as UFOMOD. As an example the countermeasures submodule of UFOMOD, Ver NE 87/1, was chosen.

A Latin hypercube sampling design code is used to generate a set of different input parameter values for running UFOMOD. A graphics program produces CCFDs and estimated confidence bands. The variability of consequences with respect to changes in uncertain input parameter values is evaluated by a sensitivity analysis code, providing partial rank correlation coefficients (PRCCs) and percentage contributions (so - called 'coefficients of determination', R^2) of uncertain model parameters to variations in consequence values. Thus the ranked influence of the uncertain parameters on the different consequence types could be shown.

Examples of input and output of the uncertainty codes and the graphics program are given.

This user guide shall complement, but not substitute, the corresponding detailed user guides of the original uncertainty and sensitivity codes.

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