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Guidelines for Uncertainty Analysis

developed for the participants in the BIOMOVS II study

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BIOMOVS - an international study to test models designed to predict the environmental transfer and bioaccumulation of radionuclides and other trace substances

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Preface

BIOMOVS II (BIOspheric MOdel Validation Study - Phase II) is an international cooperative study to test models designed to quantify the transfer and bioaccumulation of radionuclides and other trace substances in the environment.

The BIOMOVS II study is jointly managed by five organisations:

- The Atomic Energy Control Board of Canada;
- Atomic Energy of Canada Limited, AECL Research;
- Centro de Investigaciones Energéticas Medioambientales y Tecnológicas, Spain;
- Empresa Nacional de Residuos Radiactivos SA, Spain;
- Swedish Radiation Protection Institute.

This report has been produced to provide guidelines for uncertainty analysis for use by participants in the BIOMOVS II study. It is hoped that others with an interest in modelling contamination in the biosphere will also find it useful. The report has been prepared by members of the Uncertainty and Validation Working Group and has been reviewed by other BIOMOVS II participants. The opinions expressed are those of the authors and should not be taken to represent the views of the BIOMOVS II sponsors or other BIOMOVS II participating organisations.

Contents

1. Introduction

An uncertainty analysis provides a quantitative estimate of the range of model outputs that results from uncertainties in the structure of the model or the inputs to the model. If the analysis is carried out in an appropriate way, the probability will be high that the range will contain the true value (or values) that the model seeks to predict. The analysis can also be extended to identify the sources that dominate the overall uncertainty, so that priorities can be set for work aimed at reducing the uncertainty. For these reasons, uncertainty analysis is an integral and important part of simulation modelling. But if the uncertainty estimates are to be meaningful and of practical use, the analysis must be carried out systematically, with due regard to the purpose of the model, the quality of the data, and the nature of the application. The methods and assumptions used in the analysis must be clearly documented.

BIOMOVS I was the first international model evaluation program in which best estimate predictions were accompanied by a confidence interval. However, the uncertainties estimated by the various participants often differed widely in magnitude for a given scenario. Some variability is to be expected because many aspects of uncertainty analysis are largely subjective, but a part of the variation could also be explained by a lack of familiarity with the formal techniques of uncertainty analysis, and the use of different techniques by different participants at each step in the process. This made it difficult to use the results to draw conclusions regarding the agreement between models, or to know the degree of confidence that should be placed in the predictions for this set of scenarios and modellers.

The present guidelines are an attempt to bring consistency to the uncertainty analysis carried out for BIOMOVS II. They outline the steps to be followed in an uncertainty analysis, recommend methods to be used at each step, and provide practical information on implementing the methods, since there are many ways to perform an uncertainty analysis, and the methods must be chosen to match the type of model and data available, and the application in question. The intended audience for these guidelines is BIOMOVS participants, and the methodologies have been specifically chosen for use with the models and scenarios developed within the BIOMOVS program. Moreover, an attempt was made to recommend approaches that are generally familiar and accessible to participants in the study. Where appropriate, alternative methods are mentioned briefly, and references given to point readers to more in depth discussions. It is beyond the scope of this document to justify the choice of methods, or to detail their limitations.

The two main classical approaches to uncertainty analysis involve analytical methods (Cox and Baybutt 1981, Worley 1987) and statistical methods based on random (Monte Carlo) sampling (IAEA 1989). They may be applied directly to the models, or used in conjunction with techniques such as response surface replacement and differential analysis (Cox and Baybutt 1981, Iman and Helton 1988). Moreover, the application of fuzzy set theory to uncertainty analysis has recently been investigated (Shaw and Grindrod 1989). Only the approach based on Monte Carlo simulation will be discussed here. This technique is well matched to the complexity of environmental transfer models.

It is not intended that participants adhere rigidly to these guidelines. Approaches other than those recommended may be more appropriate for some applications. Also, some participants may have alternative uncertainty analysis

procedures in place. In general, participants are free to chose whatever method they feel is most suitable, keeping in mind the need to produce meaningful uncertainty estimates that can be compared with those of others. Consistency does not imply that all participants will produce uncertainty estimates that are equal in magnitude; the need to make many judgmental decisions in the analysis makes differences inevitable.

The guidelines are not meant to be comprehensive, or to replace the many excellent publications that already exist on uncertainty analysis. Rather, they attempt to summarize existing work in practical form, drawing heavily on the International Atomic Energy Agency (IAEA) Safety Series 100 (IAEA 1989) in particular. The document has been kept brief to encourage participants to read it and to use it. This has meant that many important issues associated with uncertainty analysis have not been covered. Additional information can be found in the references, or in the extensive bibliography of work on uncertainty that is appended to the guidelines. The terminology used in the guidelines conforms to the definitions given in the Glossary, which will shortly be published as a BIOMOVS II report.

It is not particularly difficult to perform an uncertainty analysis. The techniques are generally straightforward and readily accessible, through publications such as this and IAEA Safety Series 100. Moreover, there exist a number of software packages for uncertainty analysis, available either commercially or free of charge. These include TAM3 (Gardner 1988), TAMDYN (Kanyar and Nielsen 1989), TIME-ZERO (Kirchner 1989), CRYSTAL BALL (Decisioneering, Inc. 1990), and packages developed by Sandia National Laboratories (Iman and Shortencarier 1984, Iman et al. 1985) and Gesellschaft für Reaktorsicherheit (Banaschik 1992).

The techniques discussed here are applicable to (linear or nonlinear) deterministic models, where the set of mathematical expressions acting on the variables (the mathematical operator) gives the rate of change of these variables. Stochastic modelling is an alternative approach in which the mathematical operator gives the probability of change in the state of the variables per unit of time. Markov models and master equations are examples of stochastic models. Due to their larger complexity these models are frequently used without uncertainty analysis.

2. Main Steps in an Uncertainty Analysis

Uncertainty in model predictions can arise from a number of sources, including specification of the problem, formulation of the conceptual model, formulation of the computational model, estimation of parameter values, and calculation, interpretation and documentation of results. Of these sources only uncertainties due to estimation of parameter values can be quantified in a straightforward manner. The main steps in a parameter uncertainty analysis are:

i) Identify the parameters that could contribute significantly to the uncertainty in the final model prediction. Care should be exercised here not to discard potentially significant uncertainties without good cause.

ii) For each parameter, construct a probability density function (PDF) to reflect the belief that the parameter will take on the various values within its possible range.

iii) Account for dependencies (correlations) among the parameters.

iv) Propagate the uncertainties through the model to generate a PDF of predicted values.

v) Derive confidence limits and intervals from the PDF of predicted values to provide a quantitative statement about the effect of parameter uncertainty on the model prediction.

Steps (i) to (iv) are discussed in Chapters 3 to 6, and step (v) in Chapter 9. Chapter 6 also deals briefly with uncertainty analysis for a stochastic endpoint. Chapter 7 deals with sensitivity analysis, and the use of intermediate results from the uncertainty analysis to rank the model parameters according to their contribution to the overall uncertainty in the model prediction. Methods to treat uncertainties arising from environmental and cultural change are discussed in Chapter 8. The document concludes in Chapter 10 with a brief summary of the key recommendations.

Uncertainty should be considered at the beginning of a consequence assessment, when the model is first chosen or developed for the problem in question. It is then possible to match the form of the uncertainty analysis to the answer that the model seeks to address, and to the available data.

3. Sources of Uncertainty

The principal factors affecting the reliability of results from environmental transfer models can been arranged into the following classes:

(1) Specification of the problem and definition of the scenario.

(2) Formulation of the conceptual model.

(3) Formulation of the mathematical model.

(4) Estimation of parameter values.

(5) Formulation of the computer code, and calculation and documentation of results.

Sources (2) and (3) are often called model structure uncertainties. Each source is discussed in turn below.

3.1 Specification of the Problem

Uncertainty can arise at the outset of a study if the type of model, the processes to be simulated, and the parameter values to be used are not carefully chosen to match the application. Inappropriate choices could result in predictions that are correct for the problem modelled, but not relevant to the problem that was supposed to be modelled. A number of factors should be considered in interpreting the scenario:

- the intended use of the results. Modelling is done for purposes that range from licensing through assessment to emergency response, and each purpose requires a different modelling approach. For example, the predictions of screening models, which are designed to be extremely conservative, could lead to inappropriate decisions if used for emergency

response purposes where realistic predictions are desired;

- temporal resolution. The modeller must decide if time-dependent or time-integrated results are required by the scenario, and whether diurnal or seasonal effects must be considered. The simulation time and the averaging time for the parameter values must be chosen to match the desired endpoints;

- spatial resolution. The scenario will determine whether generic parameter values are sufficient, or if site specific values are needed; whether the spatial scale is local or regional; and the appropriate spatial scales for averaging the parameter values; and

- the source term. The choice of model and parameter values will depend upon the character of the release, including the facility involved (reactor or disposal site), the type of release (routine or accidental), the radionuclides involved (rate of decay, chemical behaviour) and so on.

3.2 Formulation of the Conceptual Model

A conceptual model is in this context a description of the physical, chemical and biological properties of the system in question, the pathways by which radionuclides move through the system, and the processes responsible for the movement. The description should be as complete and as appropriate to the scenario as possible, based on the information and data available, and on previous experiences with similar types of problems. The formulation of the conceptual model can lead to uncertainty in a number of ways:

- not all relevant pathways and processes may be included in the model;

- the model may contain some pathways or processes that are not relevant;

- the state of the system may be poorly known, and

- the spatial variability and the future evolution of the system are likely to be poorly understood.

3.3 Formulation of the Mathematical Model

The mathematical model expresses the conceptual model through a series of equations and parameter values. Together with input data, boundary conditions and solution algorithms, it allows quantitative model results to be generated. The structure of the mathematical model depends on the scenario in question, and on the available knowledge and data. All models are simplifications of the real system, and their formulation gives rise to uncertainty in the following ways:

- some processes may be too poorly understood to be modelled adequately;

- the available data may be too scarce to allow some processes to be modelled in detail;

- some complex processes are formulated in terms of aggregated parameters that do not describe the process well;

- empirical models may result in large errors if applied outside their range

of applicability;

- the natural spatial and temporal variability of the environment can lead to large uncertainties when predictions are made for a particular location and a given time;

- models designed for long-term predictions are subject to uncertainties due to change in the environment and in human culture and technology;

- nonlinear systems that contain many feedbacks (chaotic systems) are sensitive to external perturbations. Uncertainties can arise when modelling such systems because their dynamic response is largely unpredictable for a given set of initial conditions.

One of the simplest mathematical formulations of transfers in a system is the compartmental approach. The system is regarded as composed of simple containers (subsystems) with well mixed contents. The transfers from any one subsystem to another are frequently proportional only to the concentration in the donor subsystem. These assumptions give rise to a set of coupled first order differential equations, which can be solved using analytical methods. For smaller systems it is even possible to write down closed solutions. The theory of compartmental analysis was developed some 40 years ago for biomedical applications. It has, however, since then seen widespread use in different areas mainly because of its simplicity.

A large number of compartmental models have been developed for environmental transfer studies throughout the years. A problem here may be that modellers may be tempted to use existing models where they do not apply, for example, when the assumption that the contents of a compartment are well mixed is not valid.

3.4 Sources of Uncertainty due to Estimation of Parameter Values

Most environmental transfer models involve a large number of parameters, which describe the state of the system through which the radionuclides move, the source term, the physical and biological transfer rates and the behaviour of exposed groups of humans. The parameter values used in a given model may be uncertain for a number of reasons:

- values obtained from observational data will contain measurement errors;

- observational data on which to base input variables and parameter values may be lacking;

- many parameters are known on a purely empirical basis. Use of these parameters outside their range of applicability will result in uncertainty in the model prediction;

- many parameters are subject to large variations in time and space. Averaging done on these parameters must be consistent with the model objectives;

- macroscopic processes made up of complex lower scale processes are frequently represented by using coarse-grained or lumped parameters, which do not describe the processes well;

- data derived from laboratory experiments may be quite different from values that are applicable in the field;
- the parameter may depend upon a set of (unknown) variables, which were not kept under control when the parameter values were experimentally determined;
- inappropriate generic values may be used for a site-specific study if detailed information about the site is not available;
- the modeller may be unfamiliar with the derivation and limitations of the parameter values, and use values that are unsuitable for the purpose;
- data from which parameter values have been derived may not be relevant to the specific set of conditions addressed by the model; and
- the uncertainty in parameters describing processes that undergo environmental or cultural change can increase as the calculations are extended further and further into the future.

3.5 Sources of Uncertainty due to a Stochastic Endpoint

In the discussion so far it has been assumed that the endpoint of the calculations has been of a deterministic nature - i.e. it has a specific true value. If better and better parameter values and models were used, the results would converge towards this true value. There exist, however, situations where this is not the case, but where one is left with irreducible uncertainties in the end, simply because the endpoint is a stochastic variable. This stochastic uncertainty which is of a different nature from the deterministic uncertainty, related to parameter values, is discussed further in Chapter 6.

3.6 Formulation of the Computer Code, and Calculation and Documentation of Results

The mathematical equations representing the conceptual model are translated into a set of numerical algorithms. This set of algorithms, which constitutes the computer code, may be inconsistent with the mathematical model for a number of reasons:

- numerical approximations for solutions to mathematical equations;
- inappropriate computer programming techniques;
- errors in programming, calculating, manual copying and reporting; and
- expertise of the model user.

For the most part, these represent errors rather than uncertainties, and will have a larger impact on the accuracy of the model predictions than on their uncertainties. They can be eliminated, or greatly reduced, through standard code verification methods, including the use of software engineering tools to construct the numerical algorithms, testing numerical solutions against analytical results,

intercomparing model results, peer review, and application of a variety of software verification tools (Sheng and Oren 1990).

3.7 Discussion

In theory, all of the above sources will contribute to the overall uncertainty in a given application of a model. However, the dominant source will depend upon the application. In the case of emergency response models, which must be run in real time, incomplete and inconsistent data, particularly for the source term, will likely be the primary source of uncertainty. Similarly, parameter values are likely to cause the larger uncertainties in short-term assessments (a few tens of years or less), assuming that the modeller is well versed in the assessment question and in the model itself. For long-term assessments (hundreds or thousands of years), which must deal with changes in the environment, exposure pathways and human behaviour at times far in the future, large uncertainties will be associated with scenario interpretation, the conceptual model, and the parameter values. On the other hand, for retrospective analyses of past events, where parameter values can be optimised by fitting model predictions to observations, structural uncertainty is frequently dominant (Garcia-Olivares 1992).

Ideally, uncertainty estimates for a given model prediction should include contributions from all relevant sources. However, with the exception of parameter uncertainty, none of the various sources is easy to treat in a quantitative manner. A modeller is often unaware that he has misinterpreted a scenario, left a process out of his model, or made a mistake in calculation. There is no way to account for such errors in the uncertainty estimates, although their contribution is potentially large. Similarly, a rigorous uncertainty analysis cannot be done when a process is so poorly understood that its correct mathematical representation is in doubt.

It is recommended that uncertainty analysis done for BIOMOVS purposes be based on uncertainties in parameter analysis and - if possible - also for other sources of uncertainty. There exist standard methods for carrying out a parameter analysis (Chapters 4 - 6) which, if followed, will ensure that the results are consistent, and useful for comparing the predictions of different models. Uncertainty analysis for an endpoint that is a stochastic variable is briefly discussed in Chapter 6. Uncertainties due to model structure, and to the expertise (or lack thereof) of the user, are the subjects of special studies within BIOMOVS II. The magnitude of the uncertainties from these sources may become available as the studies progress, at least for certain cases. In some special cases it is possible to treat uncertainties due to model structure in a manner similar to that of uncertainties in parameter values, viz. when there is a finite set of different model formulations which can be assigned different probabilities. If calculations are performed for all the alternative models, and their respective output distributions are weighted together, the result is a measure of the total uncertainty. It is also possible to include the "model structure parameters" in the set of ordinary parameters in a single Monte Carlo uncertainty analysis.

Although rigorous methods for estimating uncertainties from sources other than parameter values are not available at this time, semi-quantitative approaches can be applied in some cases. These are discussed below, together with measures for keeping these uncertainties to a minimum:

(i) Specification of the problem: It is the responsibility of the individual designing the scenario to ensure that the definition is as clear and complete as possible, consistent with the study objectives. Uncertainty

estimates should be provided for any variable whose value is given in the scenario definition, whether the variable describes the state of the system or the source term. It is the responsibility of each modeller to ensure that he has interpreted the scenario correctly. Interaction between designer and modeller may be necessary to achieve these goals. The modeller should also make a conscious effort to choose models, processes and parameter values to match the objectives of the scenario.

(ii) Conceptual and mathematical models: The modeller should try to ensure that all pathways and processes of importance in the scenario have been included in the model. The mathematical representation of the conceptual model should be based on the most appropriate methods, taking into account the required level of detail and the data available. Situations may arise in which a modeller is unsure of the need to include a particular process in the model. In this case, the model can be run both with and without the process, and an uncertainty analysis done for each run. Any change in the uncertainty range from run to run will provide a semi-quantitative estimate of the contribution of the process in question to the overall uncertainty.

(iii) Code formulation and execution: Modellers should ensure that they understand the workings of the computer code, the type of data the code requires, and the behaviour of the code when applied to the scenario in question. Modellers should use the various verification tools available to ensure that the code is a faithful representation of the conceptual model, and that the mathematical equations expressing the model are correctly solved. Theoretical error terms are available for many numerical procedures, and can be employed to estimate uncertainties in the algorithms used to solve the mathematical equations.

(iv) Long-term assessments: There are special problems involved in estimating uncertainties for scenarios that extend hundreds and thousands of years into the future, because of potential changes in the environment, and in human technology and culture. It is possible to account for some of this uncertainty in the parameter distributions, which reflect the possible values of the parameters in space and time. However, more rigorous approaches to the problem have been developed, and are discussed in Chapter 8. The Reference Biosphere Working Group of BIOMOVS II is using one of these approaches, and may be able to give advice on how to quantify some aspects of the uncertainty due to environmental and cultural change as the study progresses.

4. Constructing Probability Density Functions

4.1 General Guidance

All parameters that are subject to uncertainty, and to which model predictions are sensitive, should have distributed values. This includes parameters that describe the state of the system, such as soil density, lake depth or wind speed; driving variables such as the radionuclide concentration in the source compartment; and transfer parameters such as the soil solid/liquid distribution coefficient and the soil to plant concentration ratio. Distributions for the state and driving variables should be set as part of the scenario definition, whereas distributions for the transfer parameters are the responsibility of the modeller.

The methods described below apply in either case.

The PDFs for uncertain parameters must be carefully constructed if the uncertainty estimates for the model prediction are to be meaningful. This is generally a difficult task. The data available for a given parameter are often limited in both quality and quantity. Moreover, some of the data may not be consistent with the model and its application. The process of deriving PDFs is therefore largely subjective, and requires specialised knowledge and judgement of each parameter and its database. It is best done by scientists with expertise in the discipline in question. The uncritical adoption of published distributions is not recommended, since the data seldom reflect the parameter uncertainty for a given model and application.

Principles for the formal collection and use of expert opinion have received considerable attention in recent years (Hofer 1986). The process involves a number of steps, including the selection and calibration of experts, the selection of issues, elicitation training, elicitation of opinions, synthesis of opinions, review of conclusions, and complete and clear documentation. Formal techniques have been developed to study risks of reactor operation (Hora and Iman 1989), and the Commission of the European Communities (CEC) and United States Nuclear Regulatory Commission (US NRC) are currently developing procedures to be used to quantify uncertainties in accident consequence codes. It is likely that the techniques developed in the latter study will apply to environmental transfer models as well.

The formal solicitation of expert opinion is an expensive and time-consuming procedure. In addition, consensus has not yet been reached on standard approaches. For these reasons, the formal techniques are not appropriate for the BIOMOVS study. Instead, it is recommended that informal procedures be used. In constructing their PDFs, modellers are encouraged to seek input from colleagues who are easily accessible and who are knowledgeable about the parameter in question, and about its intended use. Input from at least two individuals is preferred, with conflicting views resolved through discussion to arrive at a consensus.

Construction of a PDF for a given parameter should start by assembling values, from the literature or from personal knowledge, that are consistent with the model and the application. These values will vary because of measurement error, spatial and temporal variability, extrapolation of data from one situation to another, lack of knowledge, and so on. The role of the expert is to define a PDF that reflects the probability that the parameter will take on the various values that are within its possible range. Perhaps the most objective way to do this is by first specifying the largest and smallest values that the parameter could conceivably have, and then by specifying the degree of belief (in percentage) that the parameter value will not be larger than values selected from this range. The degrees of belief so obtained will define a cumulative distribution function from which the corresponding PDF can be deduced.

The construction of the PDF becomes more objective, and the role of the expert less important, as the amount of data for a given parameter increases. Occasionally, sufficient data will exist that the PDF can be estimated using standard statistical methods. Even here, subjective judgement plays an important role, since the data must be carefully reviewed to ensure that they are relevant to the purpose of the calculation. A large data set does not automatically imply the existence of a suitable PDF. The statistical methods are discussed more fully in Section 4.2 below.

Some general guidance is given below on the type of PDF to choose for a given amount of available data:

i) Little or no relevant data exist, and no information is available on maximum, minimum, or most probable values. In this case, the specification of PDF would be entirely arbitrary. It is recommended that calculations be carried out using different PDFs for this parameter, constructed to reflect whatever information is available. The range of results will give a rough indication of the uncertainty in the predictions arising from the lack of knowledge of this parameter. This is very like a fuzzy approach.

ii) Little relevant information exists, but maximum and minimum values can be defined. In this case, a uniform distribution is recommended, since this is the least biased assumption (Tiwari and Hobbie 1976). If the range of parameter values is large (greater than one order of magnitude), a log uniform distribution is preferred to a uniform one.

iii) Little relevant information exists, but extremes and mean or modal values can be estimated. In this case a triangular distribution represents a least biased assumption (Tiwari and Hobbie 1976). A log triangular distribution is preferred if the parameter values cover a wide range.

iv) Some relevant data exists, but cannot be represented by any standard statistical distribution. A piecewise uniform (empirical) distribution is recommended in this case. It is here that expert opinion can be most fruitfully used to set the cumulative probabilities that define the PDF.

v) A substantial amount of relevant data exists and appears to be reasonably well represented by a standard distribution (normal or log normal for example). In this case, statistical methods can be used to define the attributes of the distribution (Section 4.2). If a standard PDF is assigned to a given parameter, the PDF may have to be truncated at either its upper or lower end to eliminate physically impossible values.

vi) If a parameter can be expressed as a quotient of other variables, it is often possible to approximate its PDF with a log normal distribution.

Interactive computer programs are available that allow a set of data to be compared visually with a variety of distribution functions (Frech and O'Connor 1986, Kloos et al. 1990). The programs aid the transition from the expert's judgmental qualifications to subjective PDFs that best represent his state of knowledge about the uncertain parameters. Appendix I of IAEA (1989) contains definitions of some common distributions and mathematical expressions for their means and variances.

4.2 Statistical Methods for Deterministic Parameter Uncertainties

Assume that a set of observations has been documented for the values of a parameter in a given scenario, and that there are reasons to expect these values to be well approximated by a standard PDF. In this situation it is in general possible to obtain the statistical parameters of the PDF (mean, variance etc.) which best fit the observed data. A number of different statistical methods may be used, including the maximum likelihood method, the method of moments and the method of Bayes. The maximum likelihood method has some properties that

makes it attractive:

i) It converges to the true value of the statistical parameter as the sample size increases.

ii) It is asymptotically unbiased.

iii) Among other unbiased estimators, no other has a smaller asymptotic variance.

iv) The maximum likelihood estimator of a function of the parameter is equal to that function evaluated at the maximum likelihood estimator of the parameter.

Only the maximum likelihood method will therefore be discussed here. (BIOMOVS participants are not expected to perform calculations like these. The reason to include this piece of mathematics here is simply to give the reader a feeling of the philosophy underlying the maximum likelihood method.)

The first step is to construct the maximum likelihood function *L*, which is the mathematical expression giving the probability of finding the collection of observed data, given that the type of PDF is known. *L* is simply the product of the probabilities of achieving each of the observed data values. Then the statistical parameters of the PDF are fitted so that the probability to obtain the observed data is a maximum. The solution of this maximisation problem gives us the maximum likelihood estimators of the statistical parameters. A simple example will illustrate the reasoning:

Example: The mean and variance of a normal PDF

A parameter θ is expected to be associated with a normal PDF, and a set of n measured data are all equally probable. What is the maximum likelihood estimation of the mean and variance of the distribution?

The probability of each measured value θ_i is given by the normal distribution

$$p(\theta_i) = [2\pi\sigma^2]^{-1/2} \exp[-(\theta_i-m)^2/2\sigma^2]$$

where m and σ^2 are the mean value and variance. The probability of the set of observations $\{\theta_1, \theta_2,... \theta_n\}$ is the product of the probabilities for each individual observed value:

$$L(\theta_1,\theta_2,...,\theta_n) = p(\theta_1) \cdot p(\theta_2) \cdot ... \ p(\theta_n)$$

i.e.

$$L(\theta_1,\theta_2,...,\theta_n) = [2\pi\sigma^2]^{-n/2} \exp[-\Sigma (\theta_i-m)^2/2\sigma^2]$$

where the summation in the exponent ranges over the n measured values. We now seek the values of m and σ^2 that maximise *L*. Formally this can be done by taking the logarithm of *L*, (since the logarithm of *L* must have its maximum located at the same place as *L*), differentiating this expression with respect to m and σ^2 respectively and setting these two equations equal to 0.

Since

$$\log L(m,\sigma^2) = -n \log(2\pi\sigma^2)/2 - \Sigma (\theta_i-m)^2/2\sigma^2$$

we find that

$$d(\log L)/dm = [\Sigma (\theta_i-m)] /\sigma^2 = 0 \text{ and}$$

$$d^2(\log L)/d\sigma^2 = -n/2\sigma^2 + \Sigma [(\theta_i-m)^2]/2\sigma^4 = 0$$

which implies the following estimates

$$m = \Sigma\theta_i /n$$

$$\sigma^2 = \Sigma (\theta_i-m)^2/n$$

This is a quite simple application of the maximum likelihood principle. In general the calculations tend to be more complicated.

5. Correlation between Parameters

5.1 General Remarks

Correlations between parameters in a model, i.e. their covariations, may sometimes influence the uncertainties of the results substantially. In some cases the correlations tend to cancel the parameter uncertainties, as in a simple ratio with positively correlated parameters as numerator and denominator. Generally, however, the effect may go either way.

To a modeller it is important to master correlations for two different reasons. The first, and perhaps the most obvious one, is that if there are correlations present between model parameters, then these correlations should be incorporated in the model. The second reason is that with a good knowledge of existing parameter correlations it may sometimes be possible to reformulate the model to a more efficient form. If the model is of a "scientific" or "mechanistic" kind, then one should perhaps try to use parameters that are as uncorrelated as possible. If, on the other hand, the model is intended for assessment or forecasting, then one could sometimes reduce the uncertainties in the predictions by taking advantage of correlations by lumping parameters in a clever way.

Correlations between parameters are always caused by some underlying mechanisms, which sometimes can be very intricate. In a modelling situation two different strategies may be employed to deal with existing correlations: a simplified "statistical" one which makes use solely of the matrix of variances and covariances between the parameter, and a more cumbersome "physical" one. In the former method it is assumed that the relation between the parameters can be described simply in terms of covariances, and that these quantities are known beforehand. Any temporal relation between the parameters in the model is disregarded. A minimum of input data is required, and the computational effort

is small (the price being that some more complicated types of correlations cannot be modelled). The BIOMOVS participants are advised to use this method, which is outlined below.

When using the second strategy one instead tries to mimic the processes in nature, including any existing relations between the parameters and using conditional probability functions. This strategy relies much more on good experimental and theoretical knowledge of the system studied. If, on the other hand, the knowledge is there, much more complex parameter interplays may also be modelled. It is also worth noticing that once the conditional probabilities needed are known, a covariance matrix can easily be constructed. If only the covariance matrix is given, it is not possible to construct any of the conditional probability distributions. The data reduction that is effected in the construction of a covariance matrix inevitably leads to a substantial loss of data.

5.2 The Covariance Matrix Method, Background

Consider a system which can be represented by two parameters, X and Y. The means of both parameters (denoted <X> and <Y> respectively) are given by known probability distributions. Without limiting the scope, both these distributions can be transformed to mean 0 and variance 1. Thus,

$$<X> = <Y> = 0; \quad <X^2> = <Y^2> = 1.$$

There may also be a correlation between X and Y. Such a correlation is introduced if Y contains a fraction of X (or X a fraction of Y). We can write this as:

$$X = x; \quad Y = ax + by,$$

where x and y are (unknown) uncorrelated normalised parameters, and a and b are constants. Since <Y> = 1, we have that

$$<Y^2> = <(ax + by)(ax + by)> = a^2 <x^2> + b^2 <y^2> + 2ab<xy> = a^2 + b^2 = 1,$$

since x and y are uncorrelated. Likewise, the covariance between X and Y is found from

$$<XY> = <x\,(ax + by)> = a.$$

Thus, the covariance is simply the normalised mixture of parameter X into Y. If we now add a third parameter Z into the system, this parameter can be written as:

$$Z = cx + dy + ez,$$

where z is normalised and uncorrelated with x and y. As above we then find:

$$<Z^2> = c^2 + d^2 + e^2 = 1;$$

$$<ZX> = c;$$

$$<ZY> = ac + bd.$$

If matrix notation is used, the correlated parameters are found from

$$(X, Y, Z) = M1^* \begin{vmatrix} x \\ y \\ z \end{vmatrix} \qquad \text{where } M1 = \begin{vmatrix} 1 & 0 & 0 \\ a & b & 0 \\ c & d & e \end{vmatrix}$$

and the covariances are found in

$$M2 = \begin{vmatrix} 1 & a & c \\ a & a^2 + b^2 & ac + bd \\ c & ac + bd & c^2 + d^2 + e^2 \end{vmatrix}$$

Now there is a simple relation between the two matrices: the first one multiplied by its own transpose gives the second:

$$M2 = M1\ M1^T.$$

In those cases where this composition is possible, it is also unique apart from the sign of the diagonal elements of M1. However, since these must always be positive following the definition of M1, a unique relation exists between given covariances (in M2) and the mixing of uncorrelated parameters (in M1). Since in both matrices rows are unaffected by those further down, a straightforward elimination process will give M1 from M2.

5.3 Algorithms

This relation between M1 and M2, which of course is valid for any number of parameters, is the starting point for the covariance method to produce normally distributed, correlated values. The procedure, described in Rubinstein (1981), is the following:

1. Construct the matrix M2 from the given variances and covariances.

2. Find M1 from M2.

3. Produce a number of uncorrelated, normally distributed random values with standard deviations corresponding to the parameter uncertainties, forming the vector (x, y, z,...)

4. Left multiply this vector by M1 to produce the vector of correlated values (X, Y, Z,...). These are automatically distributed as N(0, 1) with the correct variances. Finally the known parameter mean values should be added.

A simple Pascal code for this can be found in an earlier BIOMOVS paper (Gardner 1988). Gardner extended the code to handle distributions other than normal distributions. The modified algorithm is the following:

1. Construct the correlation matrix, not the variance-covariance matrix. (If all parameters are N(0, 1) the results are unchanged.)

2. Find M1 as above.

3. Produce uncorrelated N(0, 1) values, and construct correlated N(0, 1) distributed values from these and M1 as described above.

4. Use the inverse normal density function to find the probabilities for each of these correlated values.

5. Use the parameter probability density functions to find the corresponding correlated parameter values.

This algorithm will produce parameters having not the prescribed correlations, but the same rank-order correlation as the one found in the input matrix M2.

6. Methods to Propagate Parameter Uncertainties

To find the uncertainties in the different endpoints of a model, the uncertainties in the input parameters must be propagated through the model. A good discussion of this subject is found in IAEA (1989). We will therefore here give but a very short introduction to the subject, with some emphasis only on a few points not mentioned in the IAEA publication.

6.1 Common Methods

A graphical representation of parameter uncertainty propagation is found in Figure 1 below.

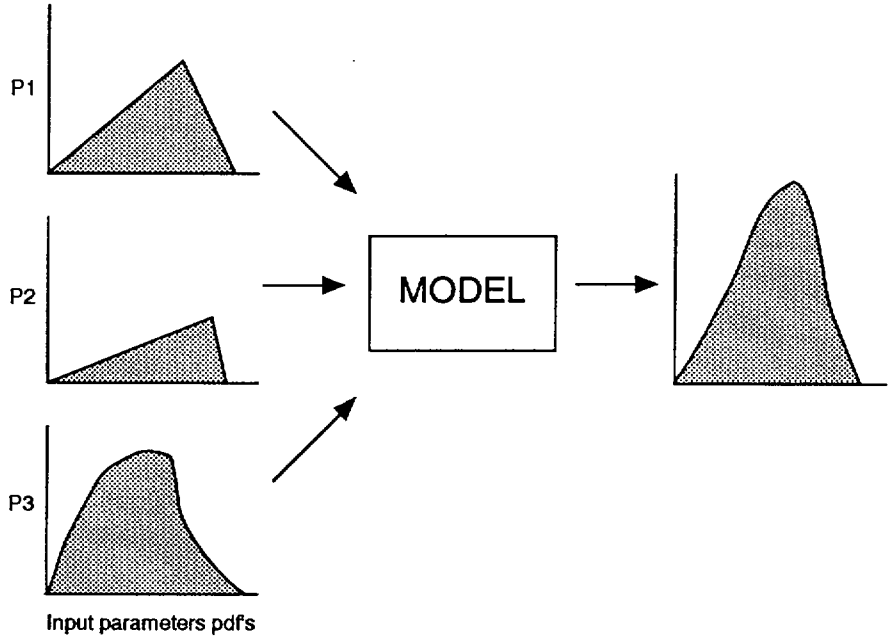


Figure 1: The propagation of input parameter density functions via the model to the resulting endpoint probability density function.

Two main classes of propagation methods can be used: analytical and numerical. Analytical methods usually provide fast results, but can only be applied to very simple models. Numerical methods, on the other hand, can be tailored to models of high complexity, but may require substantially increased computer time. For further details on analytical methods, the reader is referred to IAEA (1989) and references therein.

Numerical methods all involve choosing a number of different sets of input parameters from their PDFs, running the model for all parameter sets, and constructing PDFs for the resulting predictions from the set of individual model results. Usually the parameters are chosen at random from the input PDFs, using simple random sampling (SRS) or Latin hypercube sampling (LHS - see IAEA (1989) Appendix II for a very brief description), but systematic non-random sampling can also be used. In SRS each parameter is chosen with a probability that is solely determined by its PDF. Correlations between the parameters can be introduced as described in Chapter 5. An important merit of SRS is the fact that the resulting endpoint distributions can be seen as drawn at random from the true endpoint distributions. They can thus be used for direct statistical analysis. This is not the case if LHS is used. The merit of this technique as compared to SRS is that usually a much smaller number of samples of sets of input parameters can be used to achieve a certain variance of the endpoint distributions. This latter fact should, at least in theory, be especially marked if some of the important parameters PDFs contain long tails, i.e. if parameter values that would severely affect the resulting prediction could occur with a low probability. For SRS, reasonably stable statistics can usually be achieved from 1000 sets of input parameters; a few hundreds is usually sufficient for LHS.

The sampling strategy must be modified slightly when dealing with standard distributions that have been truncated. Each sample should initially be chosen in the normal way from the full distribution. However, if the value selected lies within the excluded ranges, it should be discarded and the distribution resampled until a value in the allowable range is chosen.

In most cases the set of input parameters chosen initially is assumed to remain constant through the entire computation. At least for short-term environmental models this may seem reasonable. It implies, however, that two important assumptions are built into the model:

i) the parameter values are time independent;

ii) there is no temporal causality in the model, i.e. intermediate results achieved during the calculations are not allowed to change the initial parameter choices.

The first of these restrictions can, at least in principle, be overcome by a change in the model parameterisation: if we know the time development of a parameter we can replace it with a time dependent expression containing time explicitly and a number of time independent new parameters.

The second restriction is much more difficult to handle. Assume as an example that you want to model a process that at some stage can go either of two completely different ways. If it goes "right", then all parameter values remain valid, but if it goes "left" the situation is so completely changed that (at least) one of the parameters in the model is no longer valid. A new value must be found, from a new PDF which may depend on the results so far, and with a completely new correlation between the changed parameter and all other

parameters. (It could be a small change such as a decrease in soil pH, or a large change such as a new ice age.) In such situations, it is clearly not possible to use an analytical approach, nor will standard numerical approaches do. It is necessary to follow the whole process over time and perform new parameter sampling, including the computation of correlations, as the time changes occur.

6.2 Uncertainty Analysis for a Stochastic Endpoint

So far it has been assumed that the parameters or variables used in the calculations, and the endpoint of the calculation itself, are of a deterministic nature - i.e. they have specific true (but unknown) values. If better and better parameter values and models could be used, the calculated endpoint would converge towards its "true" value. There exist, however, situations where this is not the case. A typical example is when health effects are calculated for individuals in a population. Even if all calculations up to and including the absorbed dose are performed with negligible uncertainties, one is left with the individual dose-effect variations, which cannot be reduced. The endpoint is stochastic.

Stochastic uncertainties in the calculations can be included on top of the deterministic results. One way to do this is to use Monte Carlo techniques. Hoffman and Hammonds (1992) describe how to proceed in a simple case. The stochastic nature of the endpoint will be reflected in the resulting cumulative or complementary cumulative distribution functions (Chapter 9). Since in this case there are no unique endpoint results, the uncertainty curves must be represented either by a number of different curves or by bands.

6.3 A Note on Random Number Generation

The so-called random numbers used in probabilistic calculations are, for practical reasons, never truly random. True random numbers cannot be software generated. Instead, one has to rely upon pseudo-random numbers - automatically generated sequences of numbers constructed to be as "random" in nature as possible. This means basically that the numbers should be generated as evenly as possible over their allowed range, that the autocorrelation in a sequence of numbers should be kept as close to zero as possible, and that the period of the number sequence (before it repeats itself) should be as long as possible.

Most pseudo-random numbers are generated using so-called linear congruent generators, in which a new number N_{i+1} is generated from the old value N_i by the recurrence relation

$$N_{i+1} = (a\, N_i + b) \bmod c$$

a, b and c are integers which, if carefully chosen, give rise to a series of pseudo-random numbers with a period equal to c. Not always, however, are the generators provided as part of different programming language compilers as good as one might expect or need. A simple algorithm to substantially upgrade the performance of the "random number" generator is the following (Knuth 1981):

Initialise

1) Set up a buffer of size n (n = 100 or so)
2) Fill this buffer with n sequential numbers from the generator
3) Generate a random index j in the interval 1 to n

Then almost uncorrelated numbers can be generated by repeating the following sequence

4) The first random number to use is the j'th value in the buffer.
5) Generate a new number from the generator and replace the value in the j'th position in the buffer with this one.
6) Linearly transform this new random number from its original range to the interval 1 to n. The transformed value is a new index j.
7) The next random number to use is the j'th value in the buffer.
8) Repeat from (5).

A source code covering this algorithm can be found in Press et al. (1989).

6.4 Generating Random Numbers from Non-uniform Distributions

If a uniform random number generator is available, it is possible to construct sequences of (pseudo) random numbers from other distributions as well.

A common procedure is to take a uniformly distributed sample along the independent axis of the inverse of the probability function F(x). Since F(x) ranges from 0 to 1, the sampling range is (0 - 1).

> Example: A random sample from a negative exponential distribution is needed. Here the normalised probability function F(x) is given by $y = F(x) = 1 - \exp(-x)$. Taking the inverse of F(x) we get
>
> $$x = -\ln(1 - y)$$
>
> If a sample of y is taken from a uniform distribution on the interval (0 - 1) the corresponding x's can be regarded as randomly sampled from an exponential distribution. (Since y is randomly distributed on (0 - 1) the expression can as well be written $x = -\ln(y)$.)

If the inverse cannot be given in a closed form (as is the case for example for the normal distribution) one may use polynomial fitted approximations. Other methods exist as well, and can be found in textbooks on probability models, such as Ross (1989).

Normally distributed random numbers are of great importance themselves, and can also be used to produce random numbers from other distributions. They may be found in different ways. If the accuracy needed is not extraordinarily high, one may use the simple algorithm

$$N = \sum_{i=1}^{12} u_i - 6$$

where the u's are uniform random numbers on the (0 - 1) interval. The random numbers N so produced will be N(0, 1) distributed.

Computer generation of random variables is treated for example in Ripley (1983).

7. Methods for Ranking Uncertain Parameters

One of the applications of an uncertainty analysis is to rank the model parameters according to their contribution to the overall uncertainty in the model prediction. This ranking may then provide a criterion to efficiently allocate further research efforts aimed at reducing the overall uncertainty. (Uncertainty analyses of environmental models often show that a few parameters explain most of the variance in the model output.)

One procedure for ranking the parameters is to do a series of Monte Carlo runs with all parameters except one varied. Repeat the exercise for the other parameters in turn. The ranking can be established by comparing the reduction in the uncertainty of the predictions from these runs with the case where all parameters were varied. Although simple in principle, this method tends to be quite tedious and expensive for more complex models, and so methods that allow a ranking without a large number of Monte Carlo simulations are desired.

This goal can be reached by basically two different approaches, depending on the model type and complexity. It can be conducted either within the framework of classical sensitivity analysis, or by applying methods of correlation and regression and using related measures of sensitivity.

7.1 Classical Sensitivity Analysis

In its simplest form, sensitivity analysis consists of varying selected input parameters, one at a time, over a specified range and recording the corresponding changes in the model predictions. Those parameters causing the largest relative changes in the predictions are defined as the important model parameters. The results may strongly depend on magnitude and direction of the perturbation in the selected input parameters.

Another disadvantage of the sensitivity approach is its local aspect, i.e. sensitivity coefficients are calculated at one point in the parameter space of the model, generally the one defined by the set of nominal (or best estimate) values of the parameters. In practice, it is necessary to evaluate sensitivity functions for several sets of input parameter values, if large variations in the inputs are to be accommodated (Cox and Baybutt 1981), leading to increased computational efforts.

The deterministic approach of differential sensitivity analysis is thus of limited use in most modelling situations. One may prefer a statistical approach which can make use of the information gathered during the propagation of the parameter uncertainties. A statistical analysis of the relationship between the selected values of the input parameters and the values of the model predictions provides measures of sensitivity in the form of correlation and regression coefficients.

7.2 Correlation and Regression Measures of Sensitivity

The statistical approach exploits the random sample of values of the input and output variables, already generated during the uncertainty propagation. The measures of sensitivity are global, since they estimate the degree of association between the output and the different input parameters over their entire sampled distributions. Sensitivity analysis is here closely related to the fitting of regression models intended to approximate the relationship between the output

and the different input parameters of the prediction model.

If the model prediction Y is a function of the parameters P_1, P_2,..., P_m, a multiple linear regression model of the following form can be constructed from a given random sample

$$(P_{1,j}, P_{2,j}, \ldots P_{m,j}, Y_j) \text{ of size n (j= 1, 2, ..., n):}$$

$$Y = a_o + a_1P_1 + a_2P_2 + \ldots + a_mP_m + \varepsilon$$

ε being the residual and the coefficients $a_o, a_1, \ldots, a_m$ being obtained according to a given criterion, which is usually the least squares criterion: minimisation of $\Sigma(Y_j - Y_j)^2$, where Y_j is the value estimated by the regression model. A commonly accepted procedure to build a regression model is the stepwise regression procedure (Draper and Smith 1966), designed to include only statistically significant variables in the model. The procedure is described in many statistical textbooks.

A convenient way to measure the adequacy of the fitted model is provided by the coefficient of determination R^2. This coefficient indicates the proportion of the variation in Y that is explained by the regression model. Different coefficients of correlation and regression can be computed, either on the values themselves or on rank-transformed values. They may be used in ranking the contribution of the different uncertain parameters to the uncertainty in the model predictions.

The coefficients a_i, i = 1, 2, ..., m of the multiple linear regression input are the partial derivatives of Y with respect to the input parameters P_i. The a_i indicate the change in Y associated with a unit change in P_i, all other P remaining constant. These regression coefficients provide therefore a measure of the sensitivity of the output to changes in the input parameters. However, since the values of the coefficients depend on the units in which the parameters are expressed, they cannot serve to measure the relative importance of the parameters. If Y and P_i are standardised according to

$$Y^* = (Y - \langle Y \rangle) / \sigma_y, \quad P_i^* = (P_i - \langle P_i \rangle) / \sigma_{xi}, \quad i = 1, 2, \ldots, m$$

where $\langle Y \rangle$ and $\langle X \rangle$ are the sample means and σ_y and σ_{xi} are the sample standard deviations, the standardised linear regression model in the standardised variables is

$$Y^* = a_1^*P_1^* + a_2^*P_2^* + \ldots + a_m^*P_m^*$$

The standardised regression coefficients (SRC) a^* indicate how many standard deviation changes in Y are associated with one standard deviation change in P_i, all other P remaining constant, and can therefore provide a measure of the relative importance of the input parameters. However, if strong correlations exist between the uncertain parameters, the standardised regression coefficients estimated from different random samples of the same size may show a large variability (IAEA 1989). The ranking is in this case less reliable than in the case of weak or no correlations.

A partial correlation coefficient (PCC) indicates the degree of linear relationship between those portions of the model prediction and the uncertain parameter that

cannot be explained by a linear relationship of each to the remaining uncertain parameters. In other words, it measures the linear relationship between the model prediction and an input parameter, with the possible linear effects of the remaining parameters removed.

The partial correlation of Y and P_i, adjusted for all P_k, $k \neq i$, may be explained as follows:

$$\text{If } Y = b_0 + \Sigma b_k P_k + \varepsilon_1 \text{ and } P_i = c_0 + \Sigma c_k P_k + \varepsilon_2$$

are linear regression models for Y and P_i in the variables P_k, k= 1, 2, ..., m, $k \neq i$, then the partial correlation coefficient of Y and P_i is the correlation coefficient of the residuals ε_1 and ε_2.

From a given random sample ($P_{1,j}$, $P_{2,j}$, ... , $P_{m,j}$, Y_j) of size n (j = 1, 2, ..., n) the sample partial correlation coefficient is obtained as the sample correlation coefficient r_{r1r2} of residuals ($\varepsilon_{1,j}$, $\varepsilon_{2,j}$), j= 1, 2, ..., n.

Both standardised and partial regression coefficient measures may be useful in ranking the importance of the input parameters. The partial coefficients measure the unique contribution of each variable, while the standardised coefficients parcel out the non-unique or shared contribution in a manner consistent with maximising the explanatory power of the regression model (Iman et al. 1985). The ranking may be based on the absolute values of either the partial derivatives of the standardised regression model or the unique contribution of the input parameters to the explanatory capability of the fitted model.

Nonlinear relationships between variables as well as extreme values may affect the ability to use the previous measures, which are based on the assumption of linearity. If the raw data are replaced by rank-transformed data, the same regression procedures can be applied on the ranks. The rank transformation tends to linearise nonlinear relationships and to reduce the effect of extreme values. However, since the procedure also eliminates the insight into the amount of variance accounted for by each parameter, it is of a somewhat limited use.

7.3 Recommendations

Although automated procedures are available nowadays to ease the implementation of classical (differential) sensitivity analysis (Horwedel et al. 1992), the use of the statistical approach is strongly advised when analyzing environmental transfer models. It uses the same information that was produced during the propagation of the parameter uncertainties, and the derived measures of sensitivity are global, since the parameters are allowed to vary over their full ranges. It is important to remember, however, that sensitivity measures derived from regression are meaningful only as long as the regression model has a high explanatory power (expressed by the coefficient of determination R^2).

Codes to perform correlation and regression analyses are found in a number of commercial statistical packages. A code for FORTRAN 77 is available from Sandia Laboratories (Iman et al. 1985). Source codes for FORTRAN, C and Pascal are described in for example Press et al. (1989). Standardised regression coefficients and partial correlation coefficients provide slightly different and complementary information, and so it can be of value to calculate both sets.

Finally, it is worth mentioning that other techniques of sensitivity analysis are emerging, like the uncertainty reduction method (Ishigami and Homma 1989), which was compared with PCC/SRC and shown to lead to close agreement (Togawa and Homma 1991). However, at the present stage, it seems too early to endorse this method and prefer it to the more established methods based on regression.

8. Specific Sources of Uncertainty in Models for Long Term Prediction

8.1 General Remarks

Some assessments require predictions to be made over very long time frames. The migration of radionuclides from a high-level waste repository through the geosphere and biosphere provides an example. High level wastes do not decay to a radioactivity level similar to that of natural uranium ores until several tens of thousands of years or so. This time scale is, therefore, sometimes used as the simulation period in assessing the fate of high level wastes. Some authors recommend that even longer time periods be considered.

Over long periods of time, processes of change are expected to occur in the biosphere, as well as in the geosphere and the repository itself. These may include:

- changes in the climate;
- changes in human activities that may affect the system, or the exposure pathways;
- changes in the transport processes; and
- structural changes in the biosphere itself.

In order to deal with such changes, it is necessary to model the evolution of the geosphere/biosphere system, to model radionuclide transport in that system, and to model possible unforeseen events and perturbations to the system. The uncertainties in the predictions of such models are large, because the evolution of the system is often poorly understood. Moreover, the uncertainties stemming from model structure, and from parameter values and input data are larger in long-term models than they are in short-term models.

The prediction of the future state of the biosphere, and of radionuclide transport through it, can be aided by studies of similar systems and processes that were active in the past. These natural analogue studies provide evidence of radionuclide transport and behaviour in evolving systems over long periods of time. Similarly, current studies on environmental changes that are presently occurring on global scales will help to guide the development of long-term models.

It is probably unrealistic to model the long-term evolution of social practices, or populations. However, some probabilistic predictions could be made of the maximum size of future populations by requiring that they be compatible with biosphere processes such as photosynthesis, the total area of arable soil, mineral resources and other economic and ecological constraints.

8.2 Long Term Models and ways to Quantify the Prediction Uncertainties

There are currently two main approaches to the description and modelling of the geosphere-biosphere system, and to estimate the uncertainties of the predictions: the scenario analysis approach (Cranwell 1990) and the environmental simulation approach (Thompson 1988, Dames and Moore 1989, Ringrose 1991).

Both approaches include events and processes. The first approach focuses mainly on events, the second approach focuses mainly on processes. A process is the action of a set of forces in a given system with a given set of boundary constraints resulting in some response of the system. Events are unpredictable phenomena affecting the system behaviour and which (i) are not effects of known processes, or (ii) are related to known processes but the relationship cannot be modelled.

Both approaches are complex and time-consuming, and require the input of a large group of experts. It is not expected that participants in most BIOMOVS scenarios will carry out such analyses, even for scenarios that extend far into the future. The methods are presented for interest and completeness, and to demonstrate the effort required to perform a rigorous uncertainty analysis in long-term models. The Reference Biosphere Working Group of BIOMOVS is using the scenario analysis approach in its work, and may be able to quantify some aspects of the uncertainty due to environmental and cultural change by the end of the study.

8.2.1 The Scenario Analysis Approach

The scenario analysis approach begins by developing a list of all events or processes believed to be relevant to the system (Bonano 1990). The list can be generated using a variety of techniques including literature review, expert opinion, a public consultation program and brainstorming sessions. The emphasis at this stage is on completeness. The list could include items such as "transport", "geological medium", "water", "thermal variations", "probability of faults", "disturbances from external systems" and so on. Parameters dealing with future populations, economics and human practices can in principle be included in this list. To aid in identifying items that were initially missed, the factors are classified in several ways, and considered from a number of different viewpoints. For example, transport may be one-dimensional, two-dimensional or three-dimensional; the geological medium may be fracture dominated, matrix dominated or a combination of the two; the water may be associated with saturated or unsaturated media or a combination; and so forth. Each of these branches can then generate another set of alternatives, which in turn can generate new sets and so on, until the degree of detail is found satisfactory. It is generally impossible to demonstrate that the list is fully comprehensive. The entire list is then screened to eliminate those events that are physically unreasonable, those that have negligible consequences and those unlikely to occur.

In the next step, events and processes are combined through failure tree analysis to obtain a set of conceivable event sequences, or "scenarios". Construction of the scenarios can be aided by the techniques used to facilitate problem-solving within groups, including forward and backward induction, value-driven generation, and analogy or antithetical-driven generation (Bonano 1990). The set of scenarios is screened using criteria similar to those applied to the list of events and processes.

Consequences for each scenario are estimated in turn, together with the

associated uncertainty. In order to combine the results from the individual scenarios into overall estimates of consequence and uncertainty, the probabilities of occurrence must be specified. These probabilities are not given by the method itself, and must be set subjectively. This is one of the most critical and difficult steps in this approach.

8.2.2 The Environmental Simulation Approach

The environmental simulation approach attempts to predict the evolution of the environment, and the transport of radionuclides through it, taking into account all the relevant processes. It begins by using historical information to define a number of discrete climatic states. The evolution of the climate is then predicted by constructing sequences of these states, taking into account their probability of occurrence and their persistence. Within each state, long-term average characteristics are assumed to remain constant, but parameter values may vary on short time scales to reflect the natural variability of the system. The time-dependent climate conditions are used to drive the evolution of other parts of the environment, by providing boundary conditions and driving forces for models of ground water flow, erosion, glaciation and so on. Radionuclides are then introduced and their transport modelled, subject to the changing state of the system through time. A large number of simulations are performed, each of which describes a different potential evolution of the climate and its effects on the environment. The results can be used to construct a probabilistic estimate of the consequences of radionuclide transport in a time-dependent system. Uncertainty estimates derived from the calculations will include uncertainties due to environmental evolution. Examples of this approach are given by Dames and Moore (1989) and Ringrose (1991).

The environmental simulation approach incorporates the effects of environmental variability on several scales. However, as with other environmental transfer models, the uncertainties due to assumptions in the conceptual model are not quantified; these uncertainties could be very large in this case.

8.2.3 Comparing the Two Approaches

The distinction between the scenario analysis and the environmental simulation approaches is not very strict. In fact, in a way, they depend on each other:

- The representativeness of the finite set of reference scenarios obtained using the first methodology must be demonstrated. This can be done through models like those used in the environmental simulation approach.

- The driving forces used by the environmental simulation models must be selected using some screening method, which in many respects resembles that of the first methodology.

Correlations among events and processes, time dependent processes and the timing of events and processes are more easily addressed by the environmental simulation approach. However, Cranwell et al. (1990) have provided insights into how these issues can be incorporated into a scenario approach.

The scenario approach has a simplicity and a structure that make it attractive as a tool in decision making. The environmental simulation approach, on the other hand, is state of the art in modelling of natural variability, geobiosphere processes etc. It can therefore be a good tool for research into sophisticated ways of modelling nature, but still be applied to practical problems.

9. Presentation of Results

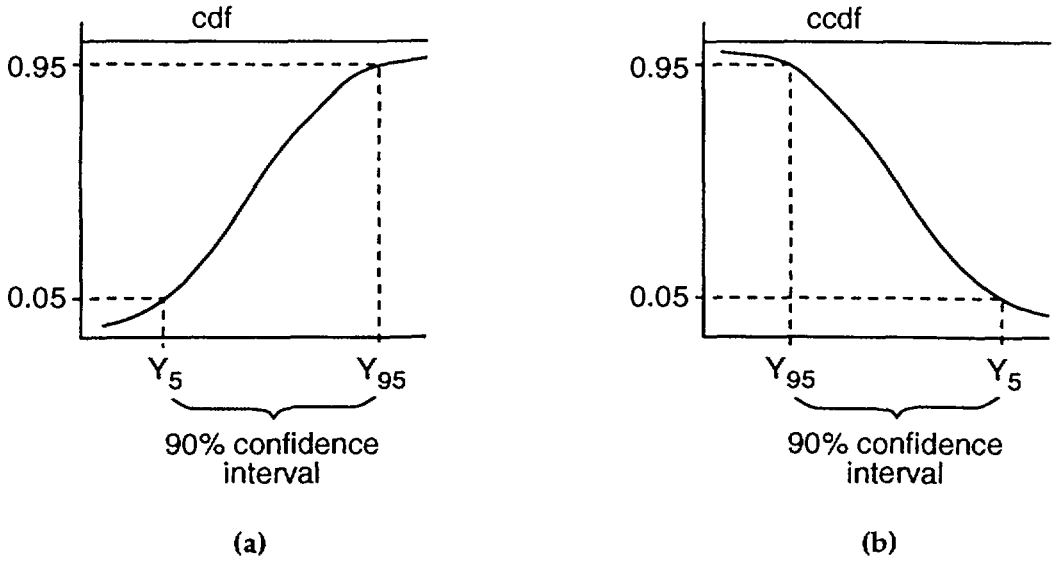
A key aspect of uncertainty analysis is documentation. The presentation of results for BIOMOVS scenarios should include quantitative statements of the uncertainties associated with model predictions, and a ranking of the parameters that contribute most to the overall uncertainty. Because of the subjective nature of uncertainty analysis, it is equally important to document clearly the methods used and the assumptions made. The following issues should be addressed in the documentation:

- what sources of uncertainty were included in the analysis;
- which model features and parameters were assigned initial uncertainties, and some comments on the validity of the estimates of these uncertainties;
- the sources of uncertainty that were not included in the calculations, both due to lack of knowledge and conceptual difficulties;
- possible differences in expert opinion connected to the uncertainty estimates;
- what parameters were correlated and how the correlation was achieved;
- how the parameter uncertainties were propagated through the model.

The final overall uncertainty for the deterministic results should be presented (in descending order of information content) as follows:

- graphically as cumulative distribution functions (cdf, Figure 2a), which show the probability $p(Y<y)$, or as complementary cumulative distributions functions (ccdf, Figure 2b), which show the probability $p(Y>y)$ (with Y the quantity of interest and y a certain level of concern). IAEA (1989) describes how to construct a cdf, or ccdf;
- graphically as the time variation of the results with the 90% confidence band if the time evolution of the system is followed (Figure 3);
- as best estimate values of the deterministic results with the uncertainty stated as 5% and 95% fractiles representing the endpoints of the 90% confidence interval;
- as upper and lower limits (in case of small sample sizes).

For judging the need for additional information and for setting priorities for further research efforts, a ranking of the uncertain parameters with respect to their contribution to the overall uncertainty should be given as explained in Chapter 7. The result of this ranking should be included in the final presentation. Here, as elsewhere, it is worth the effort to try to explain the kind of information that is hidden in the different statistics used.



Figures 2: (a) respectively the cumulative distribution function (cdf) and (b) the complementary cumulative distribution function (ccdf)

An even greater effort must be put into documentation when the analysis is undertaken for a real assessment (as opposed to a model intercomparison study such as BIOMOVS), and the results are used as input to make practical decisions regarding dose reduction, licensing, plant siting and so on. Those using the results often have little experience in the field of modelling, and may have serious problems in interpreting the results. They may have too high or too low a belief in the results, and may completely misunderstand the messages inherent in the analysis. A very important task in a complete analysis is therefore to present the results in such a way that they can be fully understood by non-experts, but at the same time be fully appreciated by the experts. The difference between (the unknown) truth, and best estimates from model calculations must be clarified. Cdf's and ccdf's contain a lot of information, and have the advantage that the confidence limits are easily read. However, these curves are notoriously difficult for non-scientists to understand, especially if they are presented with one or both axes in a nonlinear scale. Therefore they should always be followed by an explanatory text.

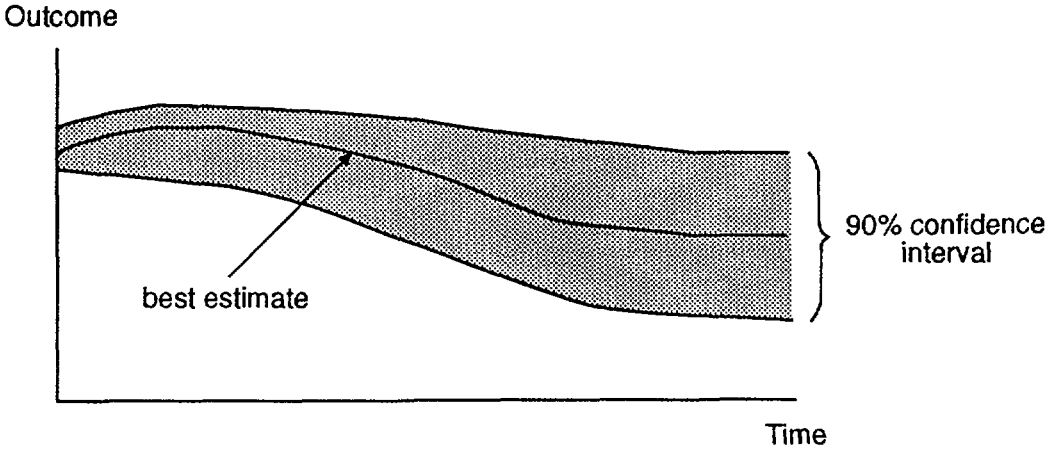


Figure 3: A way to illustrate the time development of uncertainties

The report documenting the analysis should contain both an executive summary (preferably in English, irrespective of the language of the main report) and a final concluding chapter. The closer to the final decision the reader is, the less he or she finds time to read long technical reports but instead relies on summaries. If the modeller does not produce one, someone else, less knowledgeable, may do it. The report should also include a brief discussion on the problems connected to point estimates, and the value of performing uncertainty analysis. The calculated time evolution in the system should be presented, and not endpoint results only. It may happen that significant radiological events occur at unforeseen times.

10. Summary of Recommendations

The key recommendations of this report are summarised briefly below:

- Estimate the uncertainty in all model predictions. This will allow the predictions to be used in a meaningful way.
- Choose methods of uncertainty analysis that are appropriate to the purpose of the model, the quality of the data, and the nature of the scenario.
- Try to account for all sources of uncertainty. Be aware of potential sources, even if it is not possible to quantify them. Reduce the magnitude of uncertainties that are difficult to estimate by:
  - interacting with the Working Group leader to ensure that the scenario is well defined and understood,
  - becoming familiar with the model and data to be used,
  - using software engineering techniques and computer verification tools, and
  - including all relevant processes in the model at the appropriate level of detail.
- Include in the analysis all parameters that are subject to uncertainty, and to which model predictions are sensitive.
- Use informal expert elicitation and the guidance given in Section 4.1 to construct PDFs for the uncertain parameters.
- Ensure that the data used to construct the PDFs are relevant to the endpoint of the calculations.
- Account for correlations between parameters using the covariance matrix method discussed in Chapter 5.
- Use statistical methods based on simple random sampling (Chapter 6) to propagate parameter uncertainties through the model.

- Perform a sensitivity analysis and rank the parameters according to their contribution to the overall uncertainty in the model prediction. Use both standardised regression coefficients and partial correlation coefficients (Chapter 7).

- Uncertainties due to long-term changes in the environment and in human culture and technology can be treated by the methods discussed in Chapter 8. However, because of the effort involved, it is not expected that individual BIOMOVS participants would undertake these methods.

- Express the uncertainty estimates quantitatively in terms of 90% confidence intervals (Chapter 9).

- Document in detail the methods used and assumptions made in carrying out the uncertainty analysis.

- Recognize that an uncertainty analysis is a subjective process.

The recommendations given here will not guarantee a "correct" estimate because of the many judgmental decisions required at all stages of the process. They are provided for guidance only. Participants are free to use other methods if they feel the suggestions here are inappropriate for a given application. Alternative methods should be well documented so that the results can be compared with those of others.

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12. References

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