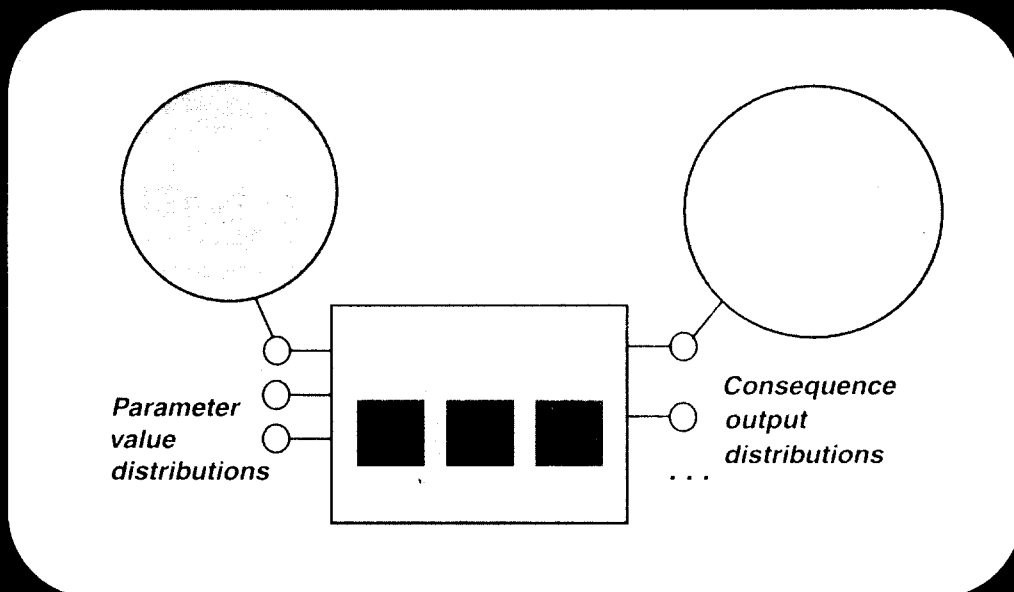




DISPOSAL OF RADIOACTIVE WASTE

THE PROBABILISTIC SYSTEM ASSESSMENT GROUP

HISTORY AND ACHIEVEMENTS
1985 – 1994



NUCLEAR ENERGY AGENCY



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ORGANISATION FOR ECONOMIC CO-OPERATION AND DEVELOPMENT**

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- *developing exchanges of scientific and technical information particularly through participation in common services;*
- *setting up international research and development programmes and joint undertakings.*

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Preface

The NEA Radioactive Waste Management Committee (RWMC), established in 1975, is an international committee of senior experts from government and industry familiar with the scientific, policy and regulatory issues in radioactive waste management. A primary objective of the RWMC is to improve the general level of understanding of waste management issues and strategies, particularly with regard to waste disposal, and to disseminate relevant information. Current NEA programmes under the RWMC focus on methodologies for the long-term safety assessment of waste disposal, and on site evaluation and design of experiments for radioactive waste disposal.

The Probabilistic System Assessment Group (PSAG) was established by the RWMC in January 1985 (originally under a different name) to help co-ordinate the development in OECD member countries of probabilistic safety assessment computer codes to be used in performance assessment of radioactive waste disposal facilities. The PSAG met approximately twice per year between its founding and its final meeting in June 1994. A key part of the Group's activities was the conduct of code intercomparison exercises aimed at building confidence in the correct operation of probabilistic assessment codes being prepared for applications in national programmes. Such exercises stimulated the thinking process and helped pave the way for basic developments, improvements and advancements in the application of probabilistic methods to assessment of waste disposal systems. In addition, the PSAG discussed many topical issues of relevance to PSA code development and to the whole question of the treatment of uncertainty in performance assessment. The PSAG reported to, and had its work reviewed by, the NEA Performance Assessment Advisory Group (PAAG).

The PSAG has been assisted by the NEA Data Bank, which undertakes the collection, testing, and dissemination of computer programs and scientific data within the NEA's fields of interest.

Acknowledgements

This report was prepared by J.E. Sinclair, Chairman of the PSAG from 1991 to 1994, and by D.A. Galson, NEA Scientific Secretary for the the PSAG from 1988 to 1991. Funding for D.A. Galson was provided by Sandia National Laboratories. Many valuable contributions and suggestions for improvement of the report were received from PSAG and PAAG members. Coordination of the various contributions and the final editing of this report was assured by C. Pescatore, NEA Scientific Secretary for the PSAG from 1991 to 1994.

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1. Introduction

The User Group for SYVAC-like Codes was set up by the Nuclear Energy Agency (NEA) in 1985, following the coming together of representatives of several national groups who were using the Canadian computer program SYVAC (SYstems Variability Assessment Code), or who were interested in applying a similar methodology. In setting up the Group under NEA sponsorship, terms of reference were agreed by the Radioactive Waste Management Committee (RWMC) of the NEA that included exchange of codes, information and experience, conducting mutual peer reviews, contributing to code justification by code comparison or other exercises, and discussing technical issues identified as being of concern for the further development of the probabilistic system assessment approach.

It soon became clear that there was interest within many of the OECD Member countries in developing probabilistic codes for the assessment of radioactive waste disposal concepts, and that such code development would not be based, in many cases, directly on SYVAC. Thus, at the end of 1985, the name of the Group was changed to the Probabilistic System Assessment Code (PSAC) User Group, to reflect the wide range of probabilistic codes being developed within an expanding membership. At the end of 1990, the name was changed again, to the Probabilistic System Assessment Group (PSAG), to reflect a broadening in the scope of the Group's activities.

Since it began, the PSAC/PSAG met approximately twice per year until 1993, with typically 15 to 30 people attending each meeting, representing 20 or more groups from at least 10 countries. The Group was assisted by a Secretariat provided by the NEA, and the NEA Data Bank gave assistance in the exchange of computer codes and the analysis of some of the exercises. The final meeting of the Group took place in June 1994.

In keeping with the aims of the Group, exchange of information and experience was accomplished through presentation at the meetings of progress reports by members, and reports on related NEA-sponsored and other international activities of relevance. Detailed exploration of important technical issues was carried out by holding Topical Sessions at most PSAG meetings. These sessions were contributed to by PSAG members and by invited speakers from outside the Group. A major part of the Group's time, however, was devoted to conducting a series of Probabilistic System Assessment Code Intercomparison exercises, known as PSACOIN exercises. These were designed to fulfil the Group's purpose of

contributing to justification of the computer codes that the participating national groups were preparing for use in safety assessments in their own national programmes. They were also important in ensuring that the Group's discussions were firmly grounded in practical application of the ideas being discussed.

Five reports documenting the results of the PSACOIN exercises have been published by the OECD. Records of the PSAG meetings, and collections of papers presented at Topical Sessions, have been distributed to Group members, and to other related NEA groups, especially the Performance Assessment Advisory Group (PAAG) and the Radioactive Waste Management Committee.

In 1989, a paper describing the objectives, achievements and the programme of activities of the PSAC/PSAG was invited by the NEA for presentation to the OECD/IAEA/CEC Conference in Paris on Safety Assessment of Radioactive Waste Repositories [Thompson et al., 1990]. This paper was prepared by several members of the Group and it, together with a booklet published in 1991 by the OECD to explain the background and progress of the PSAG [NEA, 1991], provides the basis of much of the present report. A further paper focusing on the PSACOIN exercises and their results is also available [Galson et al., 1991].

The winding up of PSAG activities reflects an increasing confidence in the practical application of PSA methodologies in OECD Member countries. For example, PSA has been used as an integral part of repository development programmes and/or actual licensing in Belgium [Marivoet, 1992; NIRAS/ONDRAF, 1994], Canada [Goodwin et al., 1994], the United Kingdom [Nirex, 1995a], and the United States [US Department of Energy, 1996].

The present report has been prepared to provide a record and summary of the achievements of the PSAG over its ten years of operation. In Chapter 2, a brief technical account of the concepts and methodology of probabilistic system assessment (PSA) is presented. A summary of the development and application of PSA around the world is given in Chapter 3. Some of the important technical issues addressed by the PSAG in its discussions and Topical Sessions are summarised in Chapter 4. Chapter 5 is devoted to the PSACOIN exercises, and summarises the content of each exercise and the conclusions reached. A summary of the achievements of the PSAG is given in Chapter 6. Chapter 7 presents an outlook on some current issues in PSA, and provides recommendations for possible future work by the international community.

2. What is PSA?

In this Report, the letters PSA are taken to stand for Probabilistic System Assessment, although the acronym is sometimes taken to represent Probabilistic Safety Assessment. A probabilistic assessment or analysis of the safety of a system could in principle use any method for evaluating the performance in which account is taken of the uncertainty that exists as to the way the system behaves, and in which that uncertainty is expressed in probabilistic terms. In the field of radioactive waste disposal, however, the term has come to be used for a particular computational approach to taking uncertainty into account. This approach, usually called the Monte Carlo method, involves repeated application of mathematical models, with some or all of the parameters of the models being given randomly selected values for each repetition.

Uncertainty enters into the long-term prediction of the performance of waste disposal systems for several reasons, including:

- The limited characterisation that can be achieved of the present state of the facility and its surroundings.
- The difficulty of extrapolating observations in time and space.
- The unpredictability of future environmental conditions and natural events that will affect system performance.
- The unpredictability of future behaviour of human beings, both as potential recipients of risks and as originators of influences on the behaviour of the system.
- Incomplete knowledge of the physical and chemical processes that combine to produce the overall behaviour of the system.
- The existence of alternative defensible models for the behaviour of parts of the system.

It is accepted that the sources of uncertainty identified above will never be completely removed and that, because of these uncertainties, any predictive modelling of system behaviour must have uncertain inputs (choice of models and assumptions, choice of data values) and, consequently, uncertain outputs (the measures of system performance). Thus,

elaborate approaches have been developed for identifying and quantifying the uncertainties in assessing the performance of waste repositories. PSA is one of these approaches and provides a means to gather and organise evidence for a judgement on the acceptability of the performance of the system in question, in view of the remaining uncertainties.

The Monte Carlo method is applied in several other fields. For some applications, for example the simulation of neutron fluxes in nuclear reactor shielding structures, the aim is to determine average patterns of behaviour in a system in which a very large number of events or processes occur, with random variation from one occurrence to another. In such cases, a Monte Carlo simulation will involve a randomly selected set of calculated cases that represents a small selection of the actual ensemble of events being modelled. In application of PSA to estimating long-term risks associated with waste disposal, the situation is rather different. There will only be one future course of the events and processes that constitute the performance of the system; the 'average' consequence is merely an agreed basis for assessing the future behaviour in the presence of uncertainty. Physically, no population of disposal systems as an ensemble of equally plausible worlds exist. However, the PSA for a disposal system assumes many (actually infinite) likely future evolutionary paths as the actual system evolution cannot be specified *a priori*. The various likely future evolutions follow specified probabilistic constraints. Therefore, the PSA should be thought of as providing a formal, explicit, and traceable procedure for considering uncertainties about the system and its parameters in developing performance estimates [cf. Watson, 1994]. In summary, a PSA cannot prove objectively how safe a radioactive waste disposal system is, but rather provides a coherent framework for incorporating expert judgement on safety relevant aspects.

A PSA necessarily includes much more than the development of equations and codes and the running of calculations. However, because the work of the PSAG focused essentially on the development, discussion and trial application of the quantitative, code-related aspects of the PSA methodology, the remainder of this chapter focuses on the mathematical aspects of Monte Carlo PSA.

2.1 The Mathematical Concepts in PSA

The mathematical principles of Monte Carlo PSA are easy to state. A system is considered whose behaviour, it is assumed, can be simulated by applying mathematical models. For an underground disposal facility for radioactive waste, the system may include the waste itself, the engineered components, such as waste packages and repository structures, and the local natural environment. The mathematical models allow the calculation of one or more measures of the performance of the system, such as the radiological dose rate at any time to an individual with given habits. Other performance measures could be the health risk corresponding to exposure to the radiological dose, the total release of activity to a specified physical boundary up to a given time, or the fraction of activity contained within a particular part of the system. Monte Carlo techniques can also be used to evaluate subsystem

performance, and some of the work within the PSAG specifically focused on subsystem calculations.

For the purpose of further discussion here, it will suffice to consider a single measure of performance, q , written as

$$q(x_1, \dots, x_k) . \quad (1)$$

This function may be quite time-consuming to compute numerically. The performance measure has here been shown as a function of several parameters, x_j , which may relate to measurable properties of system components, boundary conditions applied to the modelled region, and so on. Uncertainty about the system is expressed in terms of uncertainty about the values of the parameters, x_j . In practice, the value of a performance measure will often be calculated as a function of time, and possibly for several locations, exposure pathways, etc. This functional dependence is not shown in the notation here.

Note that some forms of uncertainty may not readily fit into the framework just described. Some mathematical models incorporate stochastic elements, whereas in expression (1) above, the performance measure is taken to be a deterministic function of its parameters. It is also possible that several defensible functional forms for q are available, constituting a further source of uncertainty about the outcome. The function q and the associated parameters, x_j , may be space and time dependent or they may depend upon other factors such as particular radionuclides under consideration. A specific example of time dependence of x_j is found in the PSA application by Her Majesty's Inspectorate of Pollution (HMIP)¹ in the UK, where models and associated parameters are dependent upon time-varying climatic conditions [Sumerling (Ed.), 1992].

The description used in probability theory to express uncertainty about a set of quantities, x_1, \dots, x_k (alternatively written as the vector \mathbf{x}), is the joint probability density function (PDF), $f(\mathbf{x})$. The probability that the true value of x_1 lies between X_1 and X_1+dX_1 , and that the value of x_2 lies between X_2 and X_2+dX_2 , and so on, is $f(\mathbf{X}) dX_1 dX_2 \dots dX_k$. In the case that all the parameters are independent (i.e., that probabilistic statements about the value of one x_j do not depend on the values of any of the other parameters), the joint PDF becomes a simple product of independent PDFs, $f_j(x_j)$:

$$f(\mathbf{x}) = f_1(x_1) f_2(x_2) \dots f_k(x_k) . \quad (2)$$

Because q depends on all the x_j via a fixed function, the value of q has an uncertainty that can also be characterised by a PDF. The aim of PSA is basically to estimate the PDF of q , the performance measure. Other equivalent ways of describing the probability distribution of q

¹ Since 1 April 1996, merged with the National Rivers Authority and Local Waste Regulatory Authorities to form the Environment Agency of England & Wales.

can be used. A common requirement is to find the expectation value (arithmetic mean) of the distribution, and other simple properties, such as percentiles.

The practical procedure of Monte Carlo PSA involves making many calculations of $q(\mathbf{x})$, using randomly sampled values of the parameters x_j . Suppose that N sample sets are taken, that in the n -th set the parameter x_j takes the value $x_j^{(n)}$, and that the performance measure takes the value:

$$q^{(n)} = q(\mathbf{x}^{(n)}) . \quad (3)$$

If all of the sampled parameter sets have been selected by a procedure that makes the expected density of sample points equal to the joint PDF $f(\mathbf{x})$, then the mean of $q(\mathbf{x})$, which is formally defined by the integral

$$\bar{q} = \int dx_1 \dots \int q(x_1, \dots, x_k) f(x_1, \dots, x_k) dx_k , \quad (4)$$

can be estimated from

$$q_e = \frac{1}{N} \sum_{n=1}^N q^{(n)} \quad (5)$$

that is, the simple mean of the q values calculated from the sample parameter values. Other simple statistics, such as the variance of q , or percentile values for the distribution of q , similarly have simple estimation formulae, usually closely related to the corresponding statistics for the finite population of sample parameter-value sets and corresponding consequence values. If the sample values $\mathbf{x}^{(n)}$ are selected with a different density than $f(\mathbf{x})$, then estimation formulae such as (5) must be modified (see the discussion of Importance Sampling under ‘Statistical sampling strategies’ in Chapter 4). It should be noted as well that, if expected values of x_j are used in equation (1), the value of q is not equal to q_e , except in the special case where the system output depends linearly on the parameters. Such nonlinear dependence on parameters is the reason for adoption of Monte Carlo or similar methods for PSA.

That probabilistic language is used to express the uncertainty in the parameter values does not imply that the physical quantities corresponding to the parameters should be considered as random. To avoid confusion, it is preferable to talk about *uncertainty* in the parameters and in the measures of performance of the system rather than about *variability* in the parameters or performance measures. From this point of view, it is perhaps unfortunate that some PSA codes have been given names including the word ‘variability’.

The term ‘variability’ is best applied to variations in time or in space of some observable quantity, such as a rock permeability. An approximate mathematical model of the system may require an average over space or time of such a quantity, or make use of other statistics

of the variation. In such a situation, if measurement is unable completely to determine the actual variations, the variability may be considered as one of the sources of uncertainty about the appropriate model parameters. Note that when this is the case, the degree of variability of the underlying quantity and the corresponding uncertainty in the model parameter will have different measures.

The random sampling process of the Monte Carlo approach is also not something that is made fundamentally necessary by the probabilistic description of the uncertainties. The mean value expressed by equation (4) above is simply an integral to be estimated, and systematic rather than randomly-sampled values of the integration variables, the x_j , could serve equally well for estimating the integral. Indeed, the simple Monte Carlo procedure is often departed from in PSA for certain purposes. For instance, it is possible to use sampling that, while still random, is biased in various ways, to achieve improved accuracy in estimating statistics such as mean values. Non-random, systematic patterns of parameter-value selection can also be used in performing sensitivity analysis (that is, testing the sensitivity of the performance measures to individual parameters or to parameter distributions).

PSA methods can be applied only to uncertainties that can be characterised in probabilistic terms. However, similar methods can be applied even when the parameter ranges considered do not derive from probability distributions. For instance, the application of Fuzzy Set Theory to characterise parameter uncertainties and corresponding consequence ranges is discussed in Chapter 4. On the other hand, some types of uncertainty that arise in assessment modelling may be difficult to describe in probabilistic terms. An example is the uncertainty about whether a particular process should be included within the conceptual model of a particular system or subsystem. PSA does not always account for such uncertainties.

2.2 Features of the Models used in Waste Disposal Applications of PSA

Whether modelling of waste disposal systems is done probabilistically or not, it is important that the construction of the mathematical models is based on a thorough analysis of all the features, events and processes that could contribute significantly to the performance of the system. As a result of such an analysis, as well as for practical reasons, the system is usually broken down conceptually into subsystems. In the part of the system in which radionuclide transport must be considered, a common breakdown is into the 'near field' (the repository, including the wastefrom and engineered barriers), the 'far field' (the geologic media constituting the primary natural barrier to radionuclide migration from the repository to the surface), and the biosphere (the surface and near-surface environment into which radionuclides may be released, giving rise to potential radiological exposure of humans). An additional subsystem is the more distant environment, whose behaviour and evolution could influence the performance of the main system. Similarly, various kinds of human influence on the main system could be considered in terms of separate subsystem models.

A further way to break down the system, and hence to structure the modelling, is according to the major pathways for radionuclide transport. Those normally considered are groundwater, repository-generated gas, human intrusion, and natural disruptive events.

Thus, the mathematical model of the whole system may need to represent a wide variety of physical, chemical and biological processes. In the near-field subsystem, it may include corrosion and other waste container failure mechanisms, dissolution of the wastefrom and other materials in groundwater, decay and in-growth of radionuclides, groundwater flow through the repository, transport of radionuclides within the repository by advection and diffusion, sorption of radioelements onto repository materials, including repository-derived complexants and colloids, and gas generation by metal corrosion or microbial action. Far-field processes modelled may include flow or percolation of water and/or gas, transport of the radionuclides by these flows and by diffusion, dissolution and transport of salt, association and dissociation of radionuclides with colloids or organic complexants, and again the decay and in-growth of the radionuclides. The biosphere processes that could be represented are numerous. In addition to the transport mechanisms present in the far field, much more complex movements of water bodies may need to be considered, along with the transport of gases, dusts, mists, and so on, and a myriad of biological processes. In addition, the biosphere modelling must account for the means of exposure of humans to the radioactivity present in the environment. Models may also be required to account for the possibility of inadvertent future human intrusion into the repository or the plume of released contaminants. Models of human exposure and human intrusion require consideration and stylised representation of human behaviour patterns, and how these could evolve in the distant future, commensurate with good radiation protection practice.

The numerical implementation of the system model may likewise involve a wide variety of methods. Many of the transport problems involve partial differential equations, whose numerical solution may be approached by finite-difference or finite-element methods, often with simplification to two dimensions or one dimension. Alternative discretization methods include network models, and models of fracture systems as stochastic distributions of planes. Some parts of the model may lend themselves to analytic solution.

In general, PSA is made more practicable if the computational models used execute very quickly on a computer, because many runs of the models must be made. To achieve this, simplifications are usually introduced. An extreme example is to eliminate all of the complexity of the biosphere, and instead use simple multiplying factors that convert radionuclide fluxes into dose rates, on the assumption of equilibrium behaviour. All simplifications should be selected and justified by comparison with more detailed deterministic modelling.

Typically, despite all simplifications, a PSA code remains a complex product. A modular structure is almost invariably adopted, whether simply by decomposition into subroutines, or by assembly of a number of semi-independent program units whose execution is managed

serially or in parallel with the aid of the computer's operating system. In either case, an 'executive' module will control the execution of specialised modules for input of the specification of the problem, random number generation for sampling of parameter values, repeated running of the model, statistical analysis of the outputs, and presentation of the results. Statistical and graphical 'post-processing' is often carried out by completely separate codes.

2.3 Analysis of PSA Results

The 'raw' output of a PSA calculation is a large amount of numerical data, consisting of a set of output quantities calculated for each of the sample cases. The set of outputs for each sample case may include several different quantities, such as release rates of activity, cumulative releases, and/or dose rates. Each quantity may be calculated for a number of different radionuclides, and may be evaluated for a range of times and for several different locations. The input data, that is the sampled values of the model parameters, should also be considered as part of the output, because it may be of interest to investigate how the outputs vary with individual model-parameter values.

The model output is of little practical use, simply as a collection of numbers. A variety of statistical analyses are therefore usually conducted. The simplest analysis is to calculate the mean value of some output quantity. Of particular note is the calculation of individual risk from the mean of the individual annual dose. An individual receiving a dose, D , in one year is reckoned to suffer a resultant risk, R , of some serious health effect (different risk measures can be defined with respect to different health effects). For small annual doses, the risk is taken to be proportional to the dose:

$$R = h D . \quad (6)$$

Values to be used for the constant of proportionality, h , are recommended by the International Commission on Radiological Protection (ICRP). Each sample case of a PSA calculation may generate, at any given time after repository closure, a different value for the annual dose. Each dose value can be associated with a conditional risk, calculated using the above formula. The overall risk must be calculated by taking the probability of each possible dose level, and multiplying by the corresponding conditional risk. If the PDF of dose, $f(D)$, were known, the overall risk could be calculated as

$$\bar{R} = \int h D f(D) dD , \quad (7)$$

that is, as h multiplied by the mean dose rate. The PSA calculation provides an estimate of the mean dose as the average of the dose values given by the set of sample cases.

Other simple statistics can be calculated from PSA results. The variance of an output quantity can be calculated as a measure of the spread of its distribution. The median of the

distribution (the value exceeded with 50% probability) is an alternative to the mean as an indicative central value. A PSA properly performed should produce a complete PDF of the performance measure(s) plus various statistics such as mean, median, and other percentiles. The term Uncertainty Analysis (UA) is used in some national programmes to apply to the determination of either the range of output or estimates of its mean and variance. The term originated when the analyses were deterministic and special procedures were adopted for UA to obtain such estimates.

A second aspect of the analysis of PSA results is Error Analysis. Statistics such as means are only estimates of the properties of the distributions of the output quantities. The true values of these statistics could only be found exactly by the Monte Carlo method if an infinite number of sample cases were taken. It is therefore important, for any given finite sample size, to have some estimate of the possible error in a calculated mean or other statistic. A widely used way to express this estimation error is to attribute a Confidence Interval to the estimate of a statistic. For instance, an estimate of a mean value may be given as $M \pm E$, at a given level of confidence, for instance 95%. This indicates that a probability of 95% can be attributed to the interval covering the true value of the mean lying within a distance E either side of the value M . In general, the interval size $\pm E$ depends on the variance of the distribution of the quantity whose mean is being estimated, the number of samples taken, and the desired level of confidence. The relationship is given in most elementary texts on statistics for the case where the sampled quantity has a Normal distribution. However, this is far from being the case for the outputs of most waste disposal system models to which PSA is applied. Rather, highly skewed distributions, in which small values are very common and large values relatively rare, are the rule.

The question of obtaining confidence intervals, without assuming anything about the shape of the distribution, was considered by the PSAG in its discussions and in conducting intercomparison exercises. In general, a confidence interval size is found using a formula of the form

$$E = \alpha S_N / N^{1/2}, \quad (8)$$

where S_N is the standard deviation of N sampled values of the output quantity. For a confidence level of 95%, the constant of proportionality, α , is approximately 1.96 if it is known that the sample mean has a Normal distribution. However, this is generally not the case in the application to waste disposal systems. A theorem due to Chebyshev leads to a value for α of approximately 4.47, based on no restrictive assumptions on the distribution of the mean estimator. However, the analysis of Woo [1989], following Guttman [1948], justifies a value for α of approximately 2.68, on the basis that the mean estimator is itself the sum of N samples from the same parent distribution. For higher levels of confidence than 95%, the difference between the Guttman and Chebyshev limits is even greater.

A third kind of analysis of PSA results is Sensitivity Analysis (SA). This means the characterisation of how sensitive the calculated results are to the uncertainty about the values of the individual input parameters, or to the details of the distributions of the parameters. The question of how SA should be performed was the subject of several discussions of the PSAG, and one intercomparison exercise (Level S) was specifically devoted to the subject (see Section 5.5). SA is an important tool in gaining understanding of complex systems. However, the strongest reason for interest in SA in the application of PSA to waste disposal safety analyses is that it can help to guide the acquisition of further data. The uncertainty in each of the model parameters used in a PSA calculation is not an inherent property, but may be reduced once sufficient information has been collected and properly interpreted, especially that from site investigation and laboratory experiments. One recent attempt to explore this problem using PSA methods has been made by Mackay [1993]. Because experiments and data collection are relatively expensive, it is important to know which parameters most sensitively affect the risks or other performance measures, so that effort to reduce uncertainty can be directed with greatest efficiency.

2.4 Presentation of PSA Results

The results of a PSA calculation carry a great deal of information, and it is important to present this information in a way that will communicate clearly. Various forms of graphical presentation are commonly used to achieve this aim. The two main objectives are to address the given regulatory limits or targets, and to provide understanding of the system being modelled.

Regulations that are framed in terms of a single output quantity, such as cumulative release to a given boundary over a given period of time, are well served by plotting the full distribution of that output quantity. One way to portray this distribution is in terms of the Complementary Cumulative Distribution Function (CCDF). The CCDF, $\bar{F}(Q)$, gives the probability that a quantity, q , is greater than any given value of Q . $\bar{F}(Q)$ is always a monotonic function, tending to value 1 as Q becomes smaller, and to value 0 as Q becomes larger. An example CCDF plot is shown in Figure 1.

If it is desired to keep separate two different kinds of contributions to the total uncertainty in q , it is possible to plot a family of CCDFs. Each single plot shows the distribution of q values arising from one class of uncertainty. The spread in the position and shape of the different CCDFs provides a portrayal of the contribution from the two classes of uncertainty. This approach is illustrated in Figure 2. Note also how the logarithmic scale for probability in Figure 2 allows greater detail to be shown in the high-release, low-probability 'tails' of the curves.

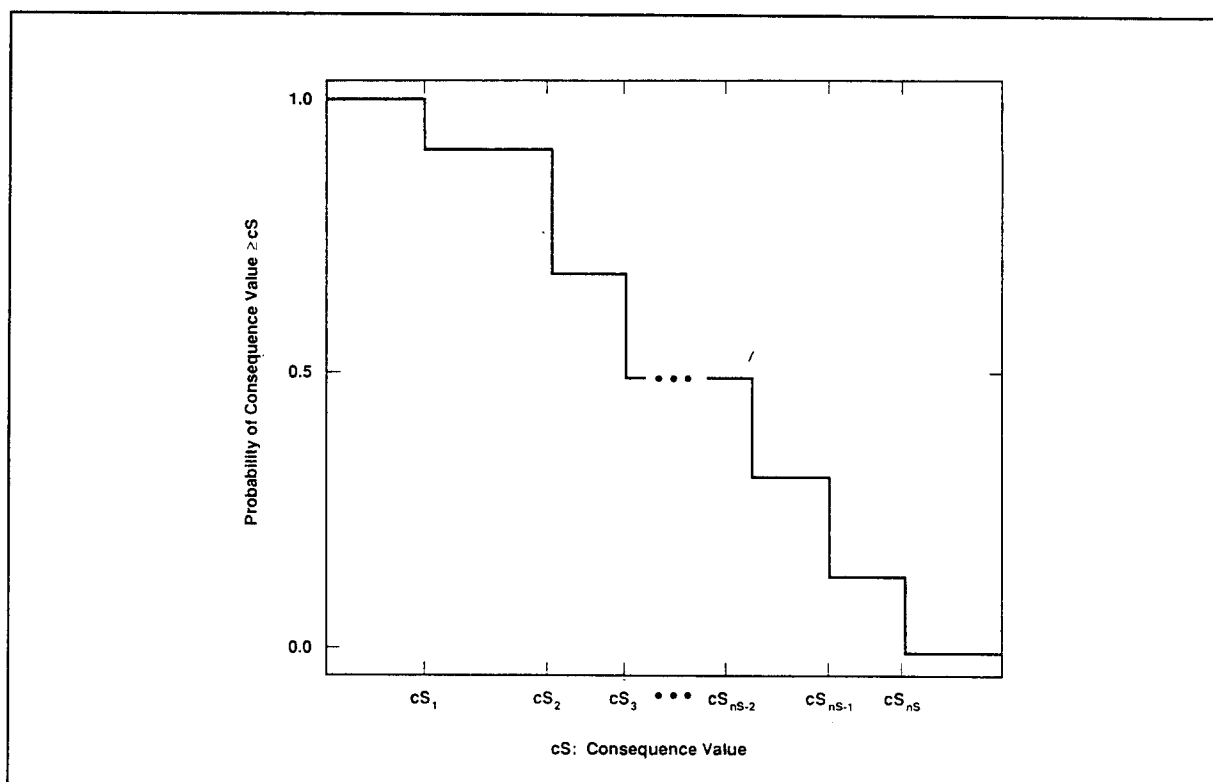


Figure 1 Illustrative plot of a Complementary Cumulative Distribution Function (CCDF) showing the probability that the calculated consequences exceed any particular value.

Regulations that are framed in terms of the mean of some quantity that depends on time, for instance annual individual dose or risk, are addressed by plotting the calculated mean(s) as a function of time. Variants of this kind of plot are useful for showing additional information. The confidence intervals associated with estimating the means can be shown using error bars, or line plots of the upper and lower interval limits (Figure 3). The contributions of different radionuclides to total dose or risk can be plotted along with the total to show clearly the way that the relative importance of the contributions varies with time.

Sensitivity analysis is concerned with the relationship between individual input and output quantities. If a given output is plotted against a single model parameter in the form of a scatter diagram, the degree and nature of any correlation between them can be made evident. Although the system model gives a well-defined functional relationship between the inputs and outputs, a plot of one output against one input quantity will show random scatter, because the results plotted include the influence of other parameters that have been randomly sampled. Figure 4 shows some examples of scatter diagrams, taken from the report of the PSACON Level 1b exercise [NEA PSAG, 1993a].

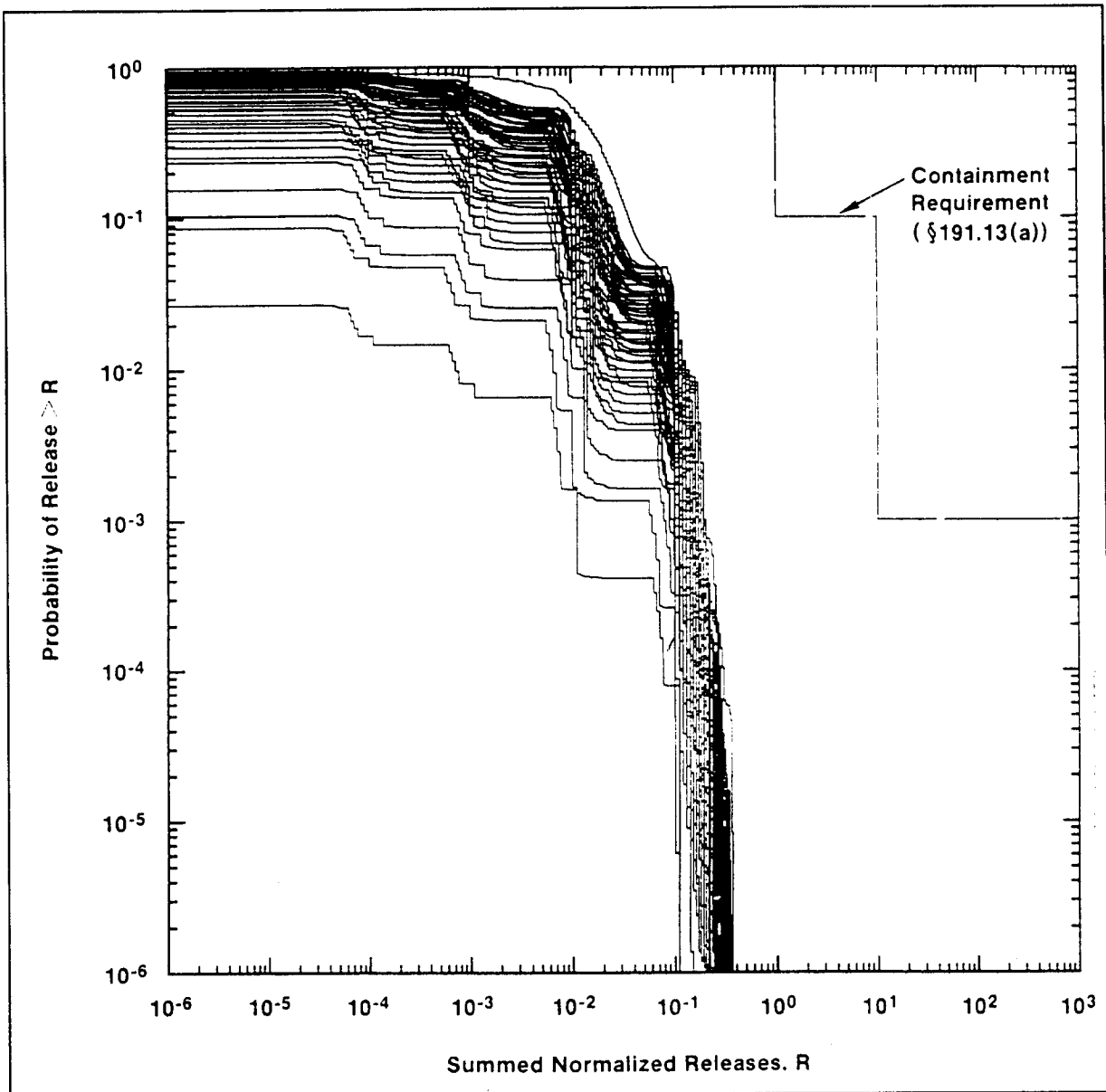


Figure 2 Distribution of CCDFs for releases to the accessible environment for one scenario class considered in the 1991 WIPP performance assessment (PA) [WIPP PA Division, 1991]. The Containment Requirement shown in the Figure forms part of the US Environmental Protection Agency's (EPA's) regulatory standard for the disposal of high-level and transuranic radioactive wastes, and is expressed as an upper limit on the probability of exceeding particular values for cumulative releases of radionuclides to the accessible environment [US EPA, 1993].

There are other ways to portray sensitivities. An interesting example is shown in Figure 5, taken from the report of the PSACON Level S exercise [NEA PSAG, 1993b], which was particularly devoted to sensitivity analysis (see Chapter 5, and also Johnson and Lucas, 1987). In this case, the departure of the plot from a straight line gives a visual indication of sensitivity.

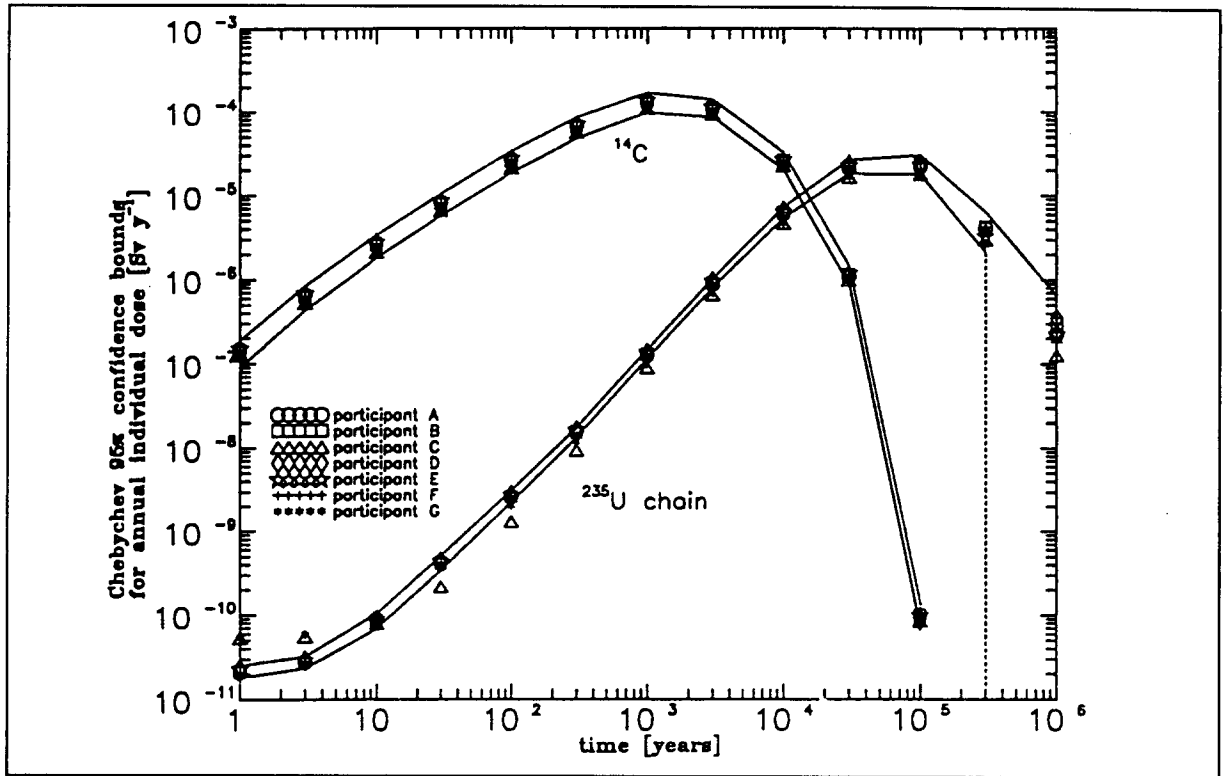


Figure 3 Example plot of mean dose versus time, taken from the PSACOIN Level 1b report [NEA PSAG, 1993a]. Results from calculations contributed by different participants in the exercise are shown using different symbols, while Chebyshev 95% confidence bounds on the mean dose values are shown using lines. Two different radionuclide contributions are shown separately. The lower limit of the 95% confidence interval is not shown for the ^{235}U chain at 10^6 years because the interval is larger than the mean value itself at this time (indicated by vertical dotted line at the last time for which the full confidence interval can be shown).

To obtain this diagram, the cases of the PSA calculation are first sorted into ascending order by the sampled value of one of the model parameters ('FLOWV1' in the example shown in Figure 5). The horizontal axis of the graph is the cumulative distribution function (CDF) for the parameter. So, for instance, the CDF value 0.60 refers to the smallest 60% of the sampled values of the parameter. For any such fraction, the calculated values of the output quantity (in this case, dose at a particular time) for those cases are summed, to give their contribution to the mean of the output quantity. This is plotted vertically, normalised so as to give the contribution relative to the mean over all cases. From Figure 5, it can thus be seen that the 20% largest sampled values of the variable FLOWV1 contributed about 80% of the mean of the dose at 10^6 years, making this dose value quite sensitive to this particular model parameter. For a parameter that was not a sensitive determinant of dose, the plot would approximate to a straight line.

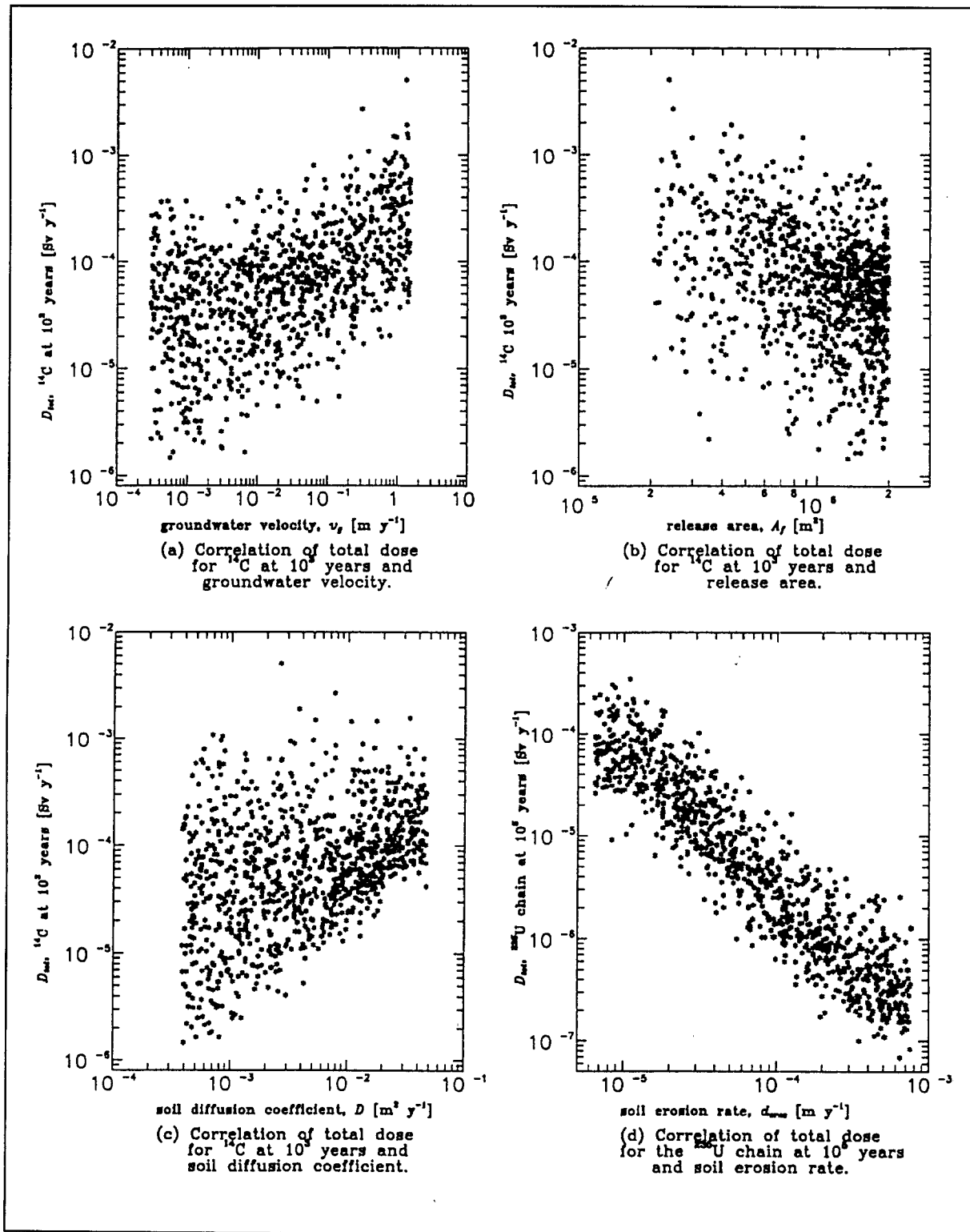


Figure 4 Example scatter plots showing the correlation between sensitive model parameters and outputs of the model, in this case the contribution of particular radionuclides to dose at particular times. The plots show a great deal of scatter, except for the d_{eros} for the ^{235}U chain at 10^5 years, which has a rank correlation coefficient of -0.94. Plots are reproduced from the PSACOIN Level 1b report [NEA PSAG, 1993a].

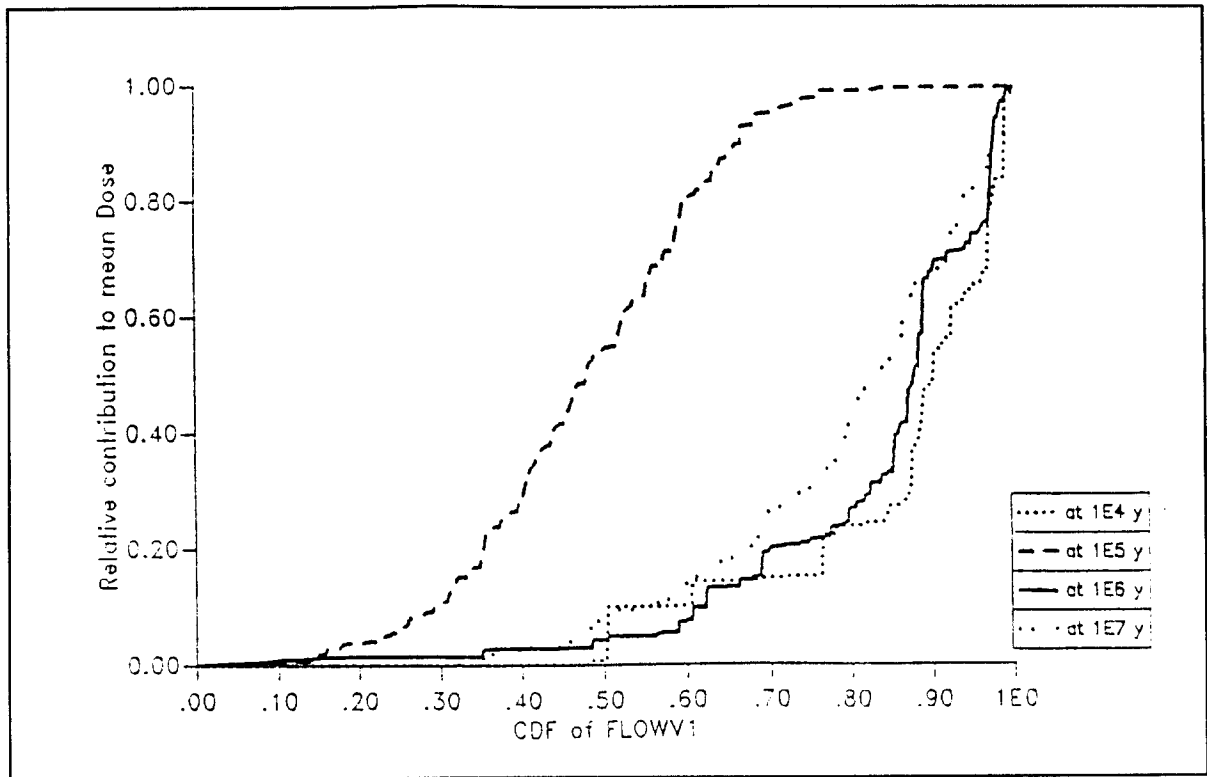


Figure 5 Example sensitivity plot showing 'Cumulative contribution to mean', reproduced from the PSACOIN Level S exercise [NEA PSAG, 1993b]. The departures of the errors from a straight line give an indication of sensitivity to the input parameter, FLOWV1.

All of the graphical presentation forms mentioned can contribute to understanding of the system. However, further communication of the significance to overall performance of selected contributing processes, or of selected subsystems, is often sought by means of other plots. For instance, in a multi-barrier disposal system, the different barriers (e.g., primary containment, chemical conditions in the repository, engineered and natural barriers to migration) contribute with different levels of efficiency, depending on the radionuclide concerned, and on time. Measures of individual barrier performance can be devised (such as the fractions of activity contained and released at each stage), and portrayed graphically using column or pie charts. Such presentation is useful regardless of whether Monte Carlo approaches are adopted for the consequence analysis.

3. Development and Application of PSA

This chapter presents a brief history of the development of PSA for waste disposal assessments. The account is largely based on the summary provided in a recent article by Thompson and Sagar [1993], which itself builds on the summary by Thompson et al. [1990].

3.1 World-wide Development of PSA Methodology

During the late 1970s and throughout the 1980s, pioneer work on the application to radioactive waste disposal of PSA using Monte Carlo methods was undertaken in the US by Sandia National Laboratories (SNL) [summarised in Cranwell et al., 1987]. The studies were applied to hypothetical high-level waste (HLW) disposal facilities in a variety of geological settings [e.g., Bonano et al., 1990]. The program SWIFT II was developed for detailed groundwater flow modelling [Reeves et al., 1986], and results obtained with this program were used to construct a network flow model composed of one-dimensional segments. The network flow-and-transport program NEFTRAN [Olague et al., 1991] was then used in probabilistic mode to estimate radionuclide releases with account taken of parameter uncertainty.

At about the same time as work was initiated in the US, work began in Canada on SYVAC, Version 1, again with a view to evaluating the potential deep geologic disposal of HLW. Analytic solutions for the source term and for groundwater-mediated transport in one dimension were evaluated and combined numerically, using parameter values sampled from PDFs based on expert judgement [Wuschke et al., 1981].

SYVAC1 was taken up in the UK by HMIP, who adapted the program to UK-specific deep and shallow disposal concepts by providing new submodels [Thompson, 1987]. The resulting programs were named SYVAC A/C [SCICON, 1986] and SYVAC D [SCICON, 1988]. Meanwhile, separate development in Canada led to versions SYVAC 2 [Sherman et al., 1986] and SYVAC 3 [Goodwin et al., 1987], incorporating multiple source-term submodels, network geosphere transport submodels, and a compartment model of biosphere transport and radiological exposure. These programs, and the extensive databases of parameter values and distributions, were developed under appropriate Quality Assurance regimes.

During the 1980s, several European groups undertook independent development of PSA programs, including LISA, developed by the Joint Research Centre (JRC) at Ispra under the European Community's (EC) radioactive waste management research programme [Saltelli et al., 1984], EMOS, developed by the GSF-Research Centre for Health and the Environment in Germany [Storck et al., 1990], PROPER, developed by the Swedish Nuclear Fuel and Waste Management Company (SKB) [SKB, 1989], and MASCOT, developed by AEA Technology on behalf of United Kingdom Nirex Limited [Sinclair and Agg, 1994]. Many of these codes were developed in the context of co-operation and information exchange provided by the PSAC User Group, as the PSAG was then known. Further improvement of PSA capability continued into the 1990s, with organisations in Japan, North America, and throughout Europe developing and using new PSA codes.

Interest in representing the processes occurring in the biosphere, as part of PSA- modelling, varied among the national groups involved. This was largely conditioned by the regulatory frameworks being addressed. For example, US regulations for disposal of HLW consider releases of radioactivity to a notional boundary around a repository² [US EPA, 1993]. Among those interested in biosphere modelling over a long time-frame, the HMIP programme stood out in giving attention to modelling the future evolution of climatic conditions and their influence on the repository environment. This work gave rise to the TIME2 [Dames and Moore, 1986] and TIME4 [Dames and Moore, 1991; 1993] codes for generating descriptions of environmental evolution in a way that could be driven by random selection of parameters, and thus incorporated into the PSA framework. To complete the capability of conducting PSA analyses with time-dependent models, the VANDAL code was developed (in several versions) by HMIP, incorporating submodels for repository releases, groundwater flow and transport (using a network approach that could extend in three dimensions and treat time-dependent boundary conditions), and a dynamic biosphere submodel [Kane, 1992].

Consideration of the effect of possible future human actions causing releases of radioactivity or otherwise affecting system performance requires a rather different approach than that for other exposure pathways. Particular attention to this class of phenomena was given in work undertaken on behalf of the US Department of Energy (DOE) for the Waste Isolation Pilot Plant (WIPP) in New Mexico [WIPP PA Division, 1991; WIPP PA Department, 1992]. Various intrusive activities, such as exploratory drilling for hydrocarbons and mining for potash, were represented as independent sequences of events whose timings and magnitudes could be obtained by sampling from probability distributions.

² US regulations for HLW disposal are currently under revision.

3.2 Applications of PSA

The *main* applications of PSA for radioactive waste disposal in OECD Member countries active in the PSAG are briefly reviewed here. The review is not comprehensive, and focuses on work in Belgium, Canada, Germany, the UK and the US, in the period during which the PSAG was active (1985-1994). Not all OECD Member countries that developed PSA codes were active in the PSAG, and this review does not consider the work in these countries (e.g., France, Netherlands). Furthermore, some countries supported development of multiple PSA codes at different national organisations (e.g., the US), but not all of these organisations (and codes) were represented at PSAG meetings, or they may have been represented only sporadically. This review also excludes consideration of developments and applications in these organisations.

Belgium

The LISA code was adapted by the Belgian Centre for Nuclear Energy Studies (SCK/CEN) in 1985 to allow simulations of the behaviour of geological disposal systems in clay layers. The post-processor of the LISA code has also been extended, in collaboration with the JRC-Ispra, to perform various techniques for sensitivity and uncertainty analysis [Saltelli and Marivoet, 1990]. Over the past decade the codes has been applied in various performance assessments, and additional modules have been developed to describe the migration of radionuclides in the various components of repository systems.

Performance assessments of the geological disposal of reprocessing waste in the Boom Clay under the nuclear site at Mol-Dessel have been carried out in the framework of the EC projects PAGIS [Marivoet and Bonne, 1988] and PACOMA [Marivoet and Zeevaert, 1991], and as part of the UPDATING 1990 study [Marivoet, 1992]. These assessments incorporated both deterministic and probabilistic calculations; a similar approach was also applied for an assessment of the direct disposal of spent fuel in clay [Marivoet et al., 1996]. A preliminary performance assessment mainly based on probabilistic calculations has also been carried out by SCK/CEN in the framework of an evaluation of the possibilities for shallow land burial of low-level radioactive waste (LLW) in Belgium [NIRAS/ONDRAF, 1994].

Canada

A series of assessments has been made of the Canadian concept for disposal of nuclear fuel waste in a deep repository in plutonic rock in the Canadian shield. The first interim assessment [Wuschke et al., 1981] made use of the first generation of the SYVAC family of PSA codes, now known as SYVAC1, and employed a relatively simple system model, with about 30 sampled parameters. SYVAC1 was also used for assessments of seabed disposal of fuel recycling wastes [Guvanasen, 1987], and for an assessment of the disposal of intermediate-level radioactive wastes (ILW) [Guvanasen, 1985].

These experiences led to the development of SYVAC2, which was used for a second interim assessment of the Canadian concept for nuclear fuel waste [Wuschke et al., 1985]. A more detailed system model was also developed, with over 500 sampled parameters. A comparison was made between alternative waste forms, spent fuel and reprocessed fuel.

The latest generation of the SYVAC family is SYVAC3, which has formed the basis of a quantitative analysis for a post-closure assessment of a possible implementation of the Canadian disposal concept [Goodwin et al., 1994]. The accompanying models and data are known as CC3. SYVAC3 has also been used in the PSACOIN exercises, and in a study of LLW disposal options for New York State [Acres International Corporation, 1989].

Germany

The main PSA capability in Germany is represented by the EMOS code [Storck et al., 1990]. German applications of PSA have been made in several research projects, such as the EC-funded studies PAGIS [Storck et al., 1988] and PACOMA [Hirsekom et al., 1991], both of which used data from a hypothetical repository in the Gorleben salt dome. A safety study of the disposal of heat-generating waste in Germany has been reported [Buhmann et al., 1991], and a variant of the EMOS code has been used for a study of disposal of HLW in salt domes in the Netherlands [Prij et al., 1993].

During the recent review of the licence application for the Konrad LLW and ILW waste repository, probabilistic calculations for uncertainty and sensitivity analysis were carried out by the Gesellschaft für Reaktorsicherheit (GRS) on behalf of the responsible authority, in order to help evaluate the deterministic analyses used in the proponent's safety case. The groundwater travel time from the repository to the biosphere was used as a performance measure.

United Kingdom

Development of capabilities for safety assessment of radioactive waste repositories has been pursued by Nirex and by HMIP. On behalf of Nirex, AEA Technology has applied the MASCOT code [Sinclair and Agg, 1994] to comparative studies of alternative types of host geological conditions for a deep ILW and LLW repository in the UK [Sinclair, 1989], and to assessments of the Sellafield site [Nirex, 1995a]. The methodology adopted by Nirex has been described in a series of Science Reports [e.g., Nirex, 1994; Nirex 1995b].

HMIP has developed and applied their approach, which aimed at employing PSA as the central aspect of their capability, as a regulator, to critically evaluate any safety case submitted by industry for the underground disposal of solid LLW and ILW. HMIP has conducted a series of three trial assessments, termed 'Dry Runs' [Thompson and Broyd (Eds.), 1986; Gralewski et al., 1988; Sumerling (Ed.), 1992], which demonstrated post-closure assessment of repositories for LLW and ILW, hypothetically constructed in clay strata at the Harwell site. The most recent study (Dry Run 3) included collation of data,

development of conceptual models, development of numerical models, elicitation of parameter distributions, probabilistic system simulations, re-examination of high-risk cases, and an 'uncertainty and bias audit'. The most notable feature of this study was its demonstration of an approach to allowing explicitly for temporal uncertainty, by modelling environmental change and its effects on the release and transport of radionuclides. The PSA codes used were VANDAL [Kane, 1992] and TIME4 [Dames and Moore, 1991].

HMIP has also applied their methodology and codes to a post-closure assessment of a near-surface LLW disposal site operated by British Nuclear Fuels Ltd. at Drigg in Cumbria [Thompson et al., 1993]. The probabilistic risk assessment calculations used a three-dimensional network model of flow and transport, and also included an assessment of human intrusion and of gas-phase effects.

United States

PSA has played a central role in a series of assessments of the WIPP, a planned geological repository for transuranic defence wastes situated in New Mexico. The assessments have been carried out by SNL on behalf of the US DOE [WIPP PA Division, 1991; WIPP PA Department, 1992]. A scenario analysis was performed, leading to a set of features, events and processes (FEPs) that were believed, after a process of systematic enumeration and screening, to be potentially significant to system performance. Important disruptive FEPs involved future human action. Combinations of the FEPs were taken to define scenarios. For each scenario, a PSA calculation was performed that accounted for the probabilities of occurrence and sequencing of the scenario-defining events. A suite of modelling programs known as CAMCON was used. The uncertainty in the model parameters was kept separate from the uncertainty about the occurrence of the scenario-defining events, and results for consequence (cumulative release to a boundary over 10^4 years post-closure) were correspondingly presented as a family of CCDFs.

Both the US DOE [e.g., Wilson et al., 1993] and the US Nuclear Regulatory Commission (NRC) [US NRC, 1995] have conducted probabilistic assessments of the potential HLW repository at Yucca Mountain in Nevada. As for the WIPP assessments, scenarios have been constructed from disturbing influences, both human-induced and natural.

Numerous other PSAs have been conducted in the US for the disposal of radioactive wastes.

4. Topics Discussed by the PSAG

In this Chapter, a selection is presented of the topical sessions that were held by the PSAG in fulfilment of its objective to explore technical issues of mutual concern to the members. A list of the main themes covered in all of the topical sessions is provided below - some of the themes were discussed more than once. The first four issues listed (shown in italics) are presented in more detail in the subsequent sections of this Chapter. The last three issues listed are discussed at least briefly in other parts of this document, as indicated below.

- *Derivation of parameter PDFs.*
- *Statistical sampling strategies and convergence.*
- *Methods for treatment of different types of uncertainty.*
- *The treatment of spatial variability.*
- The reduction of research codes to PSAC submodels.
- Scale effects and the use of nondimensional variables.
- Treatment of model uncertainty and probabilistic validation of models.
- Presentation of results from PSA (addressed in Section 2.4).
- Techniques for sensitivity analysis (addressed in Section 5.5).
- National site-specific probabilistic safety assessments (addressed in Chapter 3).

Derivation of parameter PDFs

A topical session on the justification of PDFs for use in PSAs was held at the Fifth Meeting of the PSAG (Stockholm, June 1987). Four papers were presented, covering a wide range of issues relating to this subject [NEA, 1987]. Stephens (Canada) described the guidelines that were developed at AECL for experts whose opinions were being elicited, to define PDFs for the third major assessment of the Canadian concept for HLW disposal. He stressed that only guidelines, and not rigid rules, could be laid down. Among the reasons for this are that the

appropriate values for a parameter may depend on the way the model in which it appears is being used, and on the approximations (such as time-independence) and model biases present in the model calculations. The purpose and end-points of the assessment also have an influence.

The problem of characterising correlation between two or more uncertain parameters was discussed. No general methods were found for describing such correlation, but Liebetrau (US) presented a paper on a practical methodology for implementing specified correlations in a PSA calculation.

Two other speakers presented viewpoints on the use of subjective opinions elicited from experts. Dalrymple (UK) described the systematic approach that was being used by HMIP, while Sagar (US) described two alternative methodologies for using expert opinion – the ‘Delphi Method’, using a panel of experts, and the ‘Probability Encoding Method’, in which opinions given individually by different experts are combined using a Bayesian analysis. Common features of the different approaches to elicitation are that they involve the steps of motivating, structuring, conditioning, encoding and verifying. Both of the presentations noted that structured elicitation of expert opinion, while desirable, can consume much time and expense.

The problem of dealing with conflicting opinions from different experts was also touched upon.

Group discussion about the expense of applying systematic elicitation methodologies emphasised the importance of prioritizing parameters, so that effort could be concentrated on the most important ones. In order to do this, sensitivity analyses would be needed, as well as an agreed basis for defining ‘importance’. Discussions such as this were instrumental in bringing the Group later to conduct the PSACoin Level S exercise (see Chapter 5).

Statistical sampling strategies

In Chapter 2, it was noted that PSA need not necessarily be based on the Monte Carlo method. However, all of the experience represented by the PSAG is with methods involving random sampling of parameter values from specified PDFs. Several different sampling schemes have been used, which are briefly described here, along with the Group’s views of them. The issue of sampling was discussed at several meetings, going back to the early days of the Group, and developments continued throughout the ten years of Group activity.

For the purposes of discussion, let it be assumed that the system model has several uncertain parameters that may be considered as statistically independent, and that each of these parameters has been assigned a PDF quantifying expert opinion as to the appropriateness of using different values of that parameter with the given models and for the given application. These assigned PDFs will be called the ‘true PDFs’, to distinguish them from the distribution of sampled values used in the calculations, which may be different.

In Simple Random Sampling (SRS), each independent parameter is sampled directly from its 'true' PDF, that is, the expected density of sample points in any region is equal to the density given by the assigned PDF. Because the individual parameter PDFs combine multiplicatively (equation 2 in Chapter 2), certain combinations of parameter values, deriving from the 'tails' of several individual PDFs, will only rarely be sampled, even when the number of sample cases is large. If some rare parameter combinations give rise to large calculated consequence values, large estimation errors for consequence means or other statistics can result.

A variant of SRS is Latin Hypercube Sampling (LHS), in which an attempt is made to minimise fluctuations of the actual sampling density for each parameter away from the 'true' PDF. This is done by partitioning the range of each parameter into a number of equally probable discrete sub-ranges, and arranging the sampling so that each subrange is represented exactly once for each parameter.

Another method used by some PSAG member groups is Importance Sampling (IS). This was first described for application in PSA for radioactive waste disposal systems by Johnson and Lucas [1987]. Here, the sampling process is similar to that in SRS (no restriction on representation of sub-ranges as in LHS), except that the PDFs from which the samples are drawn are different from the 'true' PDFs. The differences between the 'true' and sampling PDFs are determined in a way that aims to improve the accuracy, for a given number of sample cases, of estimation of the mean of a given output quantity. In effect, IS focuses on a particular part of 'parameter space' that is most important in determining the mean of the output quantity of interest. To compensate for the bias in the sampling, the estimation formulae for means and other statistics have to be modified.

SRS, LHS and IS were all used in the Level E exercise (see Chapter 5). However, in that exercise, no firm conclusions could be drawn about their relative merits, because the number of independent calculations represented by participants' contributions was insufficient to indicate any systematic tendency for one scheme to produce answers closer to the exact mean than another.

The measure of performance of a sampling scheme is that the means or other statistics that are estimated from the sample cases converge rapidly to the true result as the sample size (number of cases) increases. In general the true result is unknown, and it is difficult to measure the convergence simply by watching the progress of the estimated mean or other statistic as the sample size is increased. This is because, when the distribution of some consequence value is skewed, values that are much larger than the mean can occur with low probability. By definition, such outlying values arise 'without warning' at infrequent intervals as samples are taken. The running estimate of the mean can therefore appear to stabilise, only to be significantly perturbed by a large sample output value appearing.

In the topical session at the Ninth Meeting (Albuquerque, July 1989), Iman (US) argued that, for a given number of sample cases, LHS would give convergence significantly better than that of SRS. A substantial number of users of the PSA methodology have been attracted by

the prospect of such an advantage. A theoretical demonstration that the estimation accuracy of LHS is better than or equal to that of SRS is possible in the special circumstance that the consequence depends monotonically on each of the model parameters. However, even in this case, the demonstration provides no formula for the degree of benefit.

Some evidence on the relative merit of different sampling schemes was provided in a paper presented by Robinson, Roberts and Sinclair (UK) in the topical session at the Twelfth Meeting (Paris, November 1991). The paper gave results of a comparison between sampling schemes applied to a model system similar to that used in the Level E test case. This work was based on repeating the application of each sampling scheme a large number of times. The authors showed that, for the model system under consideration:

- LHS did not perform significantly better than SRS, both schemes being slow to converge as the sample size increased, for the reason that the largest values of consequence tended to arise from a rather localised region of parameter space.
- IS gave significantly better performance than SRS or LHS (a factor of 10 on the number of samples required to attain a given accuracy). This improved performance applied to estimating means of the output quantities for which the 'focusing' of the IS was designed.
- IS can perform badly (worse than SRS or LHS) for statistical results for which it is not 'focused'.
- A modified version of Importance Sampling (MIS) could be used that kept the good performance of IS for statistics on which it is focused, while retaining adequate performance (similar to that of SRS or LHS) for results on which it is not focused.

Different treatments of uncertainty

The assessment codes used by members of the PSAG are all probabilistic in nature, and are therefore aimed at taking into account uncertainties regarding the systems to be modelled. However, the manner in which uncertainty is treated can be affected by the view taken of the nature of uncertainty. This question was discussed at several meetings, and was the subject of a topical session at the Tenth Meeting of the Group (Madrid, March 1990), where five papers were presented [NEA, 1990].

Many of the uncertainties encountered in radioactive waste disposal safety assessments arise because of a lack of precise knowledge, although that knowledge could in principle be gained by sufficient investigation of the system. Probabilistic calculations are therefore performed on the basis of subjective opinion about the outcome of those theoretically possible investigations, and the parameter PDFs are subject to potential change if further information becomes available. This can be contrasted with a situation in which the behaviour of a system could be governed by stochastic events or processes operating in the future, about which only probabilistic statements can be made today, however much investigation is carried out. This second situation is encountered, for instance, in reactor safety studies where component failure is a stochastic process. At the Madrid meeting, Hofer (Germany)

proposed classification of uncertainties into Type A (stochastic) and Type B (subjective), as an aid in conducting and presenting the results of a PSA; others questioned the value of making such a distinction.

The justification for using probability theory to manipulate subjectively specified probabilities is through the Bayesian interpretation. This was clearly presented to the Group at the Madrid meeting by Smith (UK), who explained it in terms of a betting analogy. Bets about the true outcome of any uncertain event, provided they satisfy certain elementary conditions ensuring self-consistency, can be shown to be governed by the rules of probability theory.

Others have argued for the use of approaches to handling uncertainties based on Fuzzy Set theory. At the Madrid meeting, both Shaw (UK) and Nies (Germany) presented this approach, which uses 'min-max' rules to combine elementary fuzzy belief measures, in place of using the rules of probability to combine elementary probabilities. The main objections to the Fuzzy approach were that it is not necessary (because the probabilistic approach is said to be able to handle all cases), and that there is no equivalent to Bayes' Theorem for updating prior estimates.

At the Thirteenth Meeting of the PSAG (Paris, June 1992), Robinson (UK) presented an interpretation of the Fuzzy approach as a generalisation of interval analysis, and spelled out some details of how it could be implemented using Monte Carlo methods not dissimilar to those of traditional PSA. The choice between the two approaches does not rest on any practical advantages for one or the other. Rather, it is a question of the aspects of uncertainty that an assessor wishes to address. The probabilistic approach considers how expert judgement leads to a rational bet on what the outcome will be. The Fuzzy approach considers how expert judgement constrains what the possible outcomes could be. The statement of constraint on outcome will often be rather less restrictive than appears to be given by the probability distribution for consequence that is provided by PSA, because of the way that the Fuzzy approach propagates uncertainty through the models. The relevance of the different approaches to a particular safety case may depend on the regulations being addressed.

Spatial variability

Geology is inherently heterogeneous on a range of scales. Spatial heterogeneity is of particular interest in the analysis of underground waste disposal systems, not only because of the difficulties it produces in measuring hydrogeological properties, but also because its complexity makes it desirable to model groundwater flow and radionuclide transport in a way that does not take explicit account of the spatial variations. A topical session on Treatment of Spatial Variability was held during the Fourteenth Meeting of the PSAG (Albuquerque, January 1993). A variety of technical issues and approaches for analysing and modelling spatial heterogeneity were covered [NEA, 1993].

Grindrod (UK) described work using fractal concepts to represent heterogeneity within the Culebra Dolomite at the WIPP site. He reported on the use of multi-fractal techniques for analysis of the site data. Zimmerman (US) reported on the use of spatially distributed synthetic data for transmissivity to estimate groundwater travel. He implemented geostatistically based inverse techniques, and concluded that knowledge of boundary conditions is more important than exact knowledge of the transmissivity field. De Marsily (France) gave a thorough overview of non-geostatistical techniques for representation of geological features such as fractures. He discussed Boolean models for fracture and facies generation, continuous processes with defined thresholds (such as the indicator kriging and threshold Gaussian functions), and process models. Mackay (UK) reported work in which real data (from the Harwell site) had been supplemented with synthetic data. He expressed the view that a single conceptual structural model needs to be established to determine data needs. He argued that a staged site investigation is needed to obtain a single acceptable macroscopic conceptual model. Bagtzoglou (US) presented his findings on the application of artificial neural networks, for estimating spatial distributions of hydraulic conductivity. This method was shown to be appropriate when qualitative information together with 'hard' data is to be utilised. Tompson (US) gave a presentation on the application of stochastic methods for simulating transport of contaminants in complex, physically and chemically heterogeneous porous media. Neuman (US) presented his findings on scale and information content as these pertain to subsurface flow and transport modelling and validation exercises.

This topical session succeeded in providing an overview of the state of the art in the field of stochastic methods and geostatistical treatment of spatial variability.

5. The PSACOIN Exercises

The PSACOIN exercises have consumed much of the time of the PSAG, and have led to the publication by OECD/NEA of five reports. The conduct of such exercises was envisaged from the early days of the Group.

International code verification, validation and intercomparison exercises are well-established methods for helping to increase confidence in the investigation and assessment methods employed in radioactive waste disposal. Most exercises of this type have focused on models for particular subsystems of a disposal system. Thus, INTRACOIN [Swedish Nuclear Power Inspectorate, 1984; 1986], HYDROCOIN [NEA, 1992] and INTRAVAL [NEA, 1996] have concentrated on groundwater flow and radionuclide transport through the geosphere; BIOMOVs [BIOMOVs II Steering Committee, 1996] has specialised in biosphere transport models; and geochemical and coupled geomechanical-hydrological models have been addressed by the CHEMVAL [Falck and Read, 1996] and DECOVALEX [Gros et al., 1987] exercises, respectively.

The PSACOIN series differs from these in attending to models of the entire disposal system. The participants have been distinguished, not by expertise in any particular class of physical or chemical phenomena, but by interest in and involvement with the development of probabilistic assessment tools for waste disposal systems. The aim, therefore, has not been specifically to validate models against 'real-world' behaviour, but rather to build confidence in the correct operation of what can be quite large and complex computer programs for the conduct of Monte Carlo PSA calculations. All such codes incorporate (or at least control) large numbers of submodels for different subsystems, implicitly account for particular uncertainties, and produce integrated measures of system performance.

Two problems unique to comparing probabilistic results are (i) verifying the correct operation of the underlying models, and (ii) verifying the correct application of the procedure used to treat parameter uncertainty and the way the procedure leads to estimates of uncertainty in the output quantities. If two PSA codes produce different results, it is necessary to determine whether the models themselves are operating differently, or whether the differences belong more to the set of sampled cases with randomly selected parameter values.

Work on the PSACOIN exercises began at the First Meeting of the Group. A series was envisaged in which the basic methodology, independent of the particular models, would first be tested, followed by a progression towards modelling of the kind that will be involved in real national safety assessments. Because of this envisaged pattern of increasing complexity and realism, the exercises were named as 'Level X', where X was to be numeric. As the series progressed, however, certain exercises to address particular issues were devised, and non-numeric Level names were added.

After initial conception of each exercise, the usual pattern for carrying it forward was to appoint a Task Group to draw up a written specification and a questionnaire for eliciting contributions in a standard form. This work typically involved pilot running of the test case to discover any difficulties inadvertently introduced by the draft specification. With the support of the NEA, the Task Group analysed the responses, and drew up a written report for publication by the OECD. At every stage of this process, approval from the whole PSAG was obtained and, in many cases, participants iteratively updated their contributions in the light of questions raised by the Task Group's analysis. In some instances, the Task Group's analysis was able to point to errors in particular codes. A key benefit of the PSACOIN exercises was the opportunity provided for participants to become aware of and correct such errors.

In the following subsections, each of the PSACOIN exercises is described briefly.

5.1 Level 0

This first exercise aimed to test the 'executive' functions of PSA codes, including in particular the process of random selection of parameter values from different probability distributions, and the application of mathematical system models composed of linked submodels. The exercise also aimed to test 'post-processing', that is statistical analysis of the results, including sensitivity analysis. For these purposes, the exercise specified an extremely simplified model of release of radionuclides from a repository vault, one-dimensional contaminant transport through the geosphere, and doses arising from consumption of drinking water. Twelve organisations contributed results.

The 'simple' model turned out to pose certain problems for statistical convergence unlikely to be typical of real applications, but after four iterations a generally good agreement was obtained for estimates of mean dose versus time, and it was concluded that the executive parts of the PSA codes and their post-processors were operating as expected. Lessons were learned with regard to specification of exercises, analysis of results for comparison, and presentation of PSA outputs. Unresolved issues over the ranking by 'importance' of the model parameters led to the conception of further exercises.

The Level 0 report was published in 1987 [NEA PSAC User Group, 1987].

5.2 Level E

Level E shared the same purpose as Level 0, with the important addition of comparison with an exact probabilistic solution that enabled mean dose against time to be calculated precisely for a model disposal system. Needless to say, most practical assessment problems are very far from allowing such exact solutions to be obtained. Nevertheless, the model used in the exercise, while still relatively simple, was more realistic than that used for Level 0. It involved release from a vault by groundwater leaching, a two-layer geosphere transport path, and a drinking-water dose model. The exercise supplemented the probabilistic case with several deterministic cases (fixed combinations of model parameters), in order to assist with establishing correct code operation and data input. This practice was followed in later exercises.

The 'exact solution' for the mean dose against time was made possible because certain aspects of the mathematical modelling were amenable to an analytic approach. In the source term (the release rates of radionuclides from the repository), no nonlinear processes (such as solubility limitation) were specified to occur, but only simple leaching by a constant flux of groundwater was assumed, giving radionuclide fluxes proportional to the remaining inventory. Similarly, each of the two geosphere layers was treated in one dimension, with advection and longitudinal dispersion occurring in a uniform groundwater flow field, and with a simplifying choice of boundary conditions. The drinking-water dose model consisted of only a multiplying factor, which converted radionuclide concentrations in groundwater at a particular point to doses. These simplifications allowed an analytical solution to be obtained for any given choice of submodel parameters, via application of a Laplace transform to the time dimension. The PDFs for the submodel parameters were given sufficiently simple forms that averaging of the Laplace-transformed solution over the parameter distributions could also be done analytically. The only step requiring numerical evaluation was the final inversion of the Laplace transform to give mean dose as a function of time. This step could be carried out to give results that were accurate to some four decimal places, and certainly suffered no uncertainty associated with limited sample-set size.

In the exercise, participants were asked to apply their Monte Carlo PSA codes to the problem, ignoring the analytic route to the solution. Different participants tackled the problem using different parameter sampling schemes (SRS, LHS, IS), so there was an opportunity to compare whether these choices had any influence on the proximity of the results to the exact solution.

At the time the exercise was being framed, the issue of convergence of PSA results was a matter for debate within the PSAG. A proposed approach (the 'Shapiro-Wilkes' test) to testing the validity of specifying confidence limits on estimates of mean values was recommended to participants for evaluation.

The different predictions obtained with the 10 participating PSA codes were found to agree generally very well with the exact solution and with each other, despite the use of different sampling methods, different time-step algorithms, and sample sizes ranging from 100 to 10,000.

The study was inconclusive about the relative merits of different parameter sampling schemes which, if nothing else, indicated the absence of any overwhelming advantage of any one scheme for this particular problem. The Shapiro-Wilkes test was not found to be a reliable indicator of convergence. However, the exercise was useful in providing an occasion to explore the assignment of confidence limits on the basis of Normal statistics, Chebyshev's theorem, and the Guttman analysis (see Chapter 2 for a brief explanation).

The Level E report was published in 1989 [NEA PSAC User Group, 1989].

5.3 Level 1a

The Level 0 and Level E exercises had required most participants to write special-purpose code to implement the models specified. Level 1 encouraged a trend to greater realism by encouraging the use of production submodels already developed by participants for use in their national programmes.

The Level 1a test case addressed a deep repository concept: it specified modelling of mobilisation of radionuclides within the vault, release into a two-stage geosphere transport path, and calculation of doses from drinking well water. One aim of the exercise was to begin to evaluate the relative importance of the uncertainties associated with imprecisely known parameter values and those associated with the possibility of taking different mathematical approaches to modelling a given set of processes. This aim could only partially be fulfilled, because the test-case specification was fairly prescriptive with regard to geosphere transport modelling methods, although it gave more freedom with respect to the vault modelling. Modelling was also constrained in some cases by the participant's choice to use existing PSA submodels not necessarily ideally suited for this particular application, as opposed to developing new code as in previous exercises.

In the event, modelling differences mainly arose in the treatment of advective and diffusive mechanisms for the transport of radionuclides out of the repository. However, for this particular exercise, parameter value uncertainty contributed with equal or greater significance to the overall uncertainty in assessment results. Overall, the Task Group concluded that to make a more instructive comparison of the effects of parameter-value uncertainty and modelling uncertainty would require an exercise in which the modelling approaches were constrained only by the existence of a body of data (whether real experimental data or synthetic field data created for an exercise), which would serve to justify or rule out any particular modelling approach.

The Level 1a report was published in 1990 [NEA PSAC User Group, 1990].

5.4 Level 1b

The Level 1b test case contrasted with previous exercises in focusing on biosphere modelling, to the extent of excluding modelling of the geosphere altogether. Earlier exercises had used simple equilibrium biosphere models, calculating individual doses by application of radionuclide-dependent constant factors to the calculated rate of release of each radionuclide from the geosphere. Doses in the previous exercises were assumed to arise only through consumption of drinking water.

In Level 1b, a simple compartment model was used to represent transport processes within the biosphere, and seven different exposure pathways were considered in arriving at the total dose that an individual could receive. A simple source term (the rates of release of radionuclides into the biosphere) was specified, which did not seek to represent in any significant detail processes involved in release from a repository and transport through the geosphere. This specification could be considered as representing approximately some concepts for near-surface disposal, but no use was made in the exercise of such a conceptual framework.

The exercise specification was prescriptive with regard to the mathematical representation, and did not give an opportunity to compare different interpretations or treatments of a common body of information. Rather, the objectives of the exercise were to give participants experience in the application of PSA methodology to biosphere transport and exposure submodels, and to explore the effects of parameter uncertainty in these submodels, in the context of a system where individuals can be exposed by several pathways. To the extent that the codes used by participants were applicable to other systems, the exercise would also usefully contribute to the verification of these codes.

Comparison of the contributions obtained from participants, using a number of different codes, showed good agreement in general, not only for the probabilistic results, but for a deterministic 'central case' in which every parameter was fixed at a value central to the PDF defining its uncertainty. The exercise provided a demonstration of the practicability of incorporating into PSA models representations of biosphere processes with a modest level of complexity. The advantages of so doing include being able to allow explicitly for the influence of, and the uncertainty in, a number of processes within the biosphere that may interact in a complex way.

The results illustrated several effects that may arise in PSA applications incorporating moderately complex biosphere models, depending on the system being modelled:

- The peak mean dose calculated in the probabilistic case was about 5 times greater than the peak dose in the deterministic central case. Whereas the deterministic peak dose has a

probability close to one (close to being certain), the probabilistic peak dose has a much lower probability of being realised. This difference points towards the difficulty in defining a central case (for deterministic analysis) that would be equivalent to a probabilistic case (e.g., mean case) in some sense.

- Doses were not found to be significantly sensitive to any single model parameter. The uncertainty in dose arose from the combined effect of many parameter uncertainties.
- The drinking water pathway for radiological exposure, which is in many applications the only one considered, was not the most important pathway in the system studied in this exercise. The relative importance of the various exposure pathways was found to vary as a function of time.
- The timescales for redistribution of activity in the biosphere system studied were found to be long (in excess of 10^4 years). Such long timescales indicate the potential importance of representing transport within the biosphere in system assessment models, rather than relying on an equilibrium assumption and simply representing the relationship between flux released from the geosphere and dose received via a given pathway as a time-independent multiplying factor.
- There was evidence that the nature of the interface between the geosphere and the biosphere requires careful consideration. Unrealistic specification of the boundary conditions could lead to inaccurate calculation of concentrations in the biosphere.

The Level 1b report was published in 1993 [NEA PSAG, 1993a].

5.5 Level S

This purpose of this exercise was to explore approaches to sensitivity analysis in the context of PSA calculations. The exercise was not concerned with system modelling itself, as in previous exercises, but with the post-processing of model outputs. A common output data set was made available to participants, to use if they wished. The model system for study was the same as that used in the Level E exercise.

Furthermore, although a quantitative set of questions formed part of the exercise, there were also more general questions about sensitivity analysis, and participants were encouraged to submit analyses of the common output data set other than those directed at answering the basic questions, as well as original ideas on the subject of sensitivity analysis in general.

In part, the Level S exercise grew out of a question that arose in many of the preceding exercises, and which was not easy to resolve. In the earlier exercises, participants were asked to rank the parameters of the system model in order of importance. The widely varying responses indicated that the seemingly simple question “which are the most important parameters of a given system model?” has no unique meaning, and can be answered in different ways.

One traditional approach to sensitivity analysis addresses the question of parameter importance with respect to a reference point in 'parameter space'. The local variation of a model output of interest in the vicinity of this point is examined as the parameter values are changed in some systematic way. Such an approach may be called 'deterministic', to contrast it with the situation in a PSA in which the parameter-value combinations are sampled randomly from the distributions that characterise their uncertainties.

In the Level S exercise, and indeed in other PSACON exercises, many participants performed sensitivity analyses based on randomly sampled parameter values either by extracting correlation coefficients between the input parameters and one or more model outputs (such as dose at a particular time), or by performing regression analyses. These approaches are closely related and can be thought of as fitting simple functional forms (e.g. linear) to the variation of the given model output quantity as the input parameters span their ranges of interest. The fits obtained depend on the parameter distributions. In the special case of very narrow distributions, a linear form in general provides a good fit, and the correlation or regression coefficients bears a simple relationship to the gradients that could be obtained from deterministic sensitivity analysis.

The Level S problem specification and questionnaire encouraged yet another approach to sensitivity analysis, termed 'distribution sensitivity analysis'. Here, the focus is on changes to the characteristics of the whole distribution of output values produced by a PSA, as changes are made to the input parameter distributions. The motivation for taking such an approach is as follows. First, safety assessments are concerned with the distribution of consequence values, or with broad characteristics of this distribution, such as mean and spread. Second, the parameter distributions are not fixed absolutely, but are potentially subject to change as site characterisation or other data gathering reduces the uncertainty in some parameter values. In order to optimise the direction of such experimental work, it is of interest to estimate how the consequence distribution characteristics, which are the end-points of a safety assessment, would be affected by changes in the distributions characterising uncertainty in the parameters.

In the model system for Level S, the 12 uncertain parameters all had either uniform or log-uniform distributions. The quantitative questions did not suggest consideration of any departures from this class of shapes, simply shifts and symmetric changes of width. The model output quantities considered were mean dose at particular times, and maxima of dose up to particular times. The questions about the sensitivity of the output distributions concerned the mean of a given dose value, and the spread of the distribution, which was typically quantified by the variance or standard deviation. In order to allow consideration of shifted input-parameter distributions, the supplied common data set included randomly sampled parameter values covering wider distributions than the specified originals. By appropriate censoring of the data set, samples could be obtained covering the original ranges and shifted ranges as required.

The exercise achieved its objective of ensuring the development of new techniques for sensitivity analysis. Where numerical agreement was to be expected between different participants' responses to specific questions, it was generally found. Ranking of variables by importance in terms of 'distribution sensitivity' was satisfactorily consistent, at least for the most influential parameters.

A major conclusion of the exercise concerned statistical error in the probabilistic sensitivity analysis. Many of the estimated output quantities cited in the contributions were subject to standard errors that exceeded the corresponding estimated quantities in size. In other words, the estimated quantities could not be significantly distinguished from zero. As with all statistics calculated from PSA results, a reduction of error is to be expected as the number of sample cases is increased. However, it appeared that a sample size adequate to estimate mean doses with sufficient accuracy for practical purposes may often be inadequate for estimation of sensitivities of the kind considered in this exercise. This outcome emphasises the need for error analysis to accompany all statistical calculations.

One question left outstanding in the Level S exercise is the appropriate way of handling what is a common characteristic of PSA calculations for waste disposal systems, that many of the sample consequence values are zero, or effectively so. Correlation or regression analyses based on ranked output values can be significantly affected by this large number of 'tied' values, which is not typical of many other applications of statistical analysis.

However, in its discussions on sensitivity analysis, the Group was made aware of significant investigations on the subject carried out by associates of the Group who were not participants in the Level S exercise. For example, Saltelli and co-workers [1990, 1992, 1993] have given considerable attention to sensitivity analysis in general, and to the problems with tied values alluded to above. Andres and Hajas [1993] have developed a new method of sensitivity analysis, known as iterated fractional factorial design (IFFD). IFFD is based, not on the ensemble of randomly sampled cases provided by a PSA, but on systematically chosen parameter-value combinations. Its particular merit appears to be in detecting parameter sensitivities reliably even when the system model has hundreds or even thousands of uncertain parameters. IFFD is of particular interest for situations where statistical error may enter strongly into sensitivity measures derived from Monte Carlo PSA calculations.

The Level S report was published in 1993 [NEA PSAG, 1993b].

5.6 Level 2

Background to undertaking the exercise

The PSACOIN Level 2 exercise was begun in 1992 after a long period of discussion within the Group regarding its purposes and content. The Group was agreed that the new exercise should represent a significant advance over previous exercises in its degree of realism, in the following senses:

- That the physical and chemical processes would be represented more accurately.
- That the models used would be those prepared for use in actual national assessment calculations.
- That the models and data would represent realistic bodies of experimental and expert-elicited information regarding a specific site.

In the previous exercises, the specifications had determined many aspects of the system to be studied - mathematical models needed to represent the system were prescribed, and the provided data values and distributions were for parameters of particular models. Participants were then often faced with a choice: they could write new submodels for their codes, to match the exercise specifications, or they could select submodels that were at hand but written for a different purpose, and use them despite departures from the conceptualisation prescribed for the exercise.

By contrast, in a real assessment situation, there is a body of information about the system, obtained by observations, experiments or other means, and those making the assessment must choose conceptual and mathematical models according to their understanding of the system, and assign values to the model parameters in accordance with their understanding of how these model parameters relate to the measured quantities.

It was particularly in these regards that a greater degree of realism was desired for the Level 2 exercise. Furthermore, by the time the exercise was finally specified, a strong international interest had arisen in the treatment of uncertainty concerning the choice of conceptual models for the system and the processes involved. An important aim of the exercise was to contribute to understanding of the possible impact of conceptual model uncertainty on assessment results, as compared to the impact from other sources of uncertainty.

The specification of the exercise

In the discussions prior to specifying the Level 2 exercise, the option was considered to base it on an artificially created data set, for example, following an approach along the lines of that presented by Mackay [1993] in his work for HMIP. Finally, however, the exercise was based on real site information, for the WIPP, a proposed repository for defence transuranic waste,

located in south-eastern New Mexico. As noted in Section 3.2, the SNL/WIPP PA Department has been conducting iterative performance assessments of the WIPP, and data and results from the 1991 assessment [WIPP PA Division, 1991] were used in the Level 2 exercise.

The exercise is based on a particular scenario for radionuclide release into the environment that was important in the 1991 WIPP PA. This scenario involves a hypothetical inadvertent penetration of the repository and an underlying pressurised brine reservoir, by an exploratory borehole drilled in the distant future when knowledge of the repository is assumed to have been lost by society. The pressurised brine moves upward to the waste panel (at a depth of some 650 m), mixes with the contents of a waste panel, and continues upward through a pre-existing second borehole. The principal aquifer overlying the proposed repository host rock is the Culebra Dolomite layer, at a depth of some 250 m. Brine contaminated by radionuclides from the repository reaching this point would be expected to mix and flow laterally with the groundwater flowing in the Culebra. This scenario is illustrated schematically in Figure 6.

Extensive field investigations have provided information about the hydraulic transmissivity of the Culebra aquifer, and the present-day head distribution. Despite this extensive data base, the spatial variation of the properties cannot be precisely determined, and this, combined with uncertainty about the transport behaviour of solutes in groundwater in the rock, make for an assessment problem involving a rich interplay between different kinds of uncertainty.

The following specific objectives were set for the Level 2 exercise:

- To assemble model treatments of a single system using a variety of conceptual models, and thus to explore the effect of conceptual model uncertainty.
- To study progressively the effect of incorporating conceptual model uncertainty into different components of the system.
- To study, for different performance measures, the relative impact of conceptual model uncertainty.
- To study methods for the derivation of PDFs for model parameters, and to explore how this process interacts with the range of conceptual models considered.

Because the potential scope of the exercise was considerably greater than any previous in the PSACOIN series, the Group decided to conduct Level 2 in stages. Stage 1 would be concerned with assessing the importance of conceptual model uncertainty with regard to the radionuclide transport component of the various modelling systems. To achieve this restriction, the required conceptual models for components other than transport were provided. In particular, a fixed conceptual model for groundwater flow and the

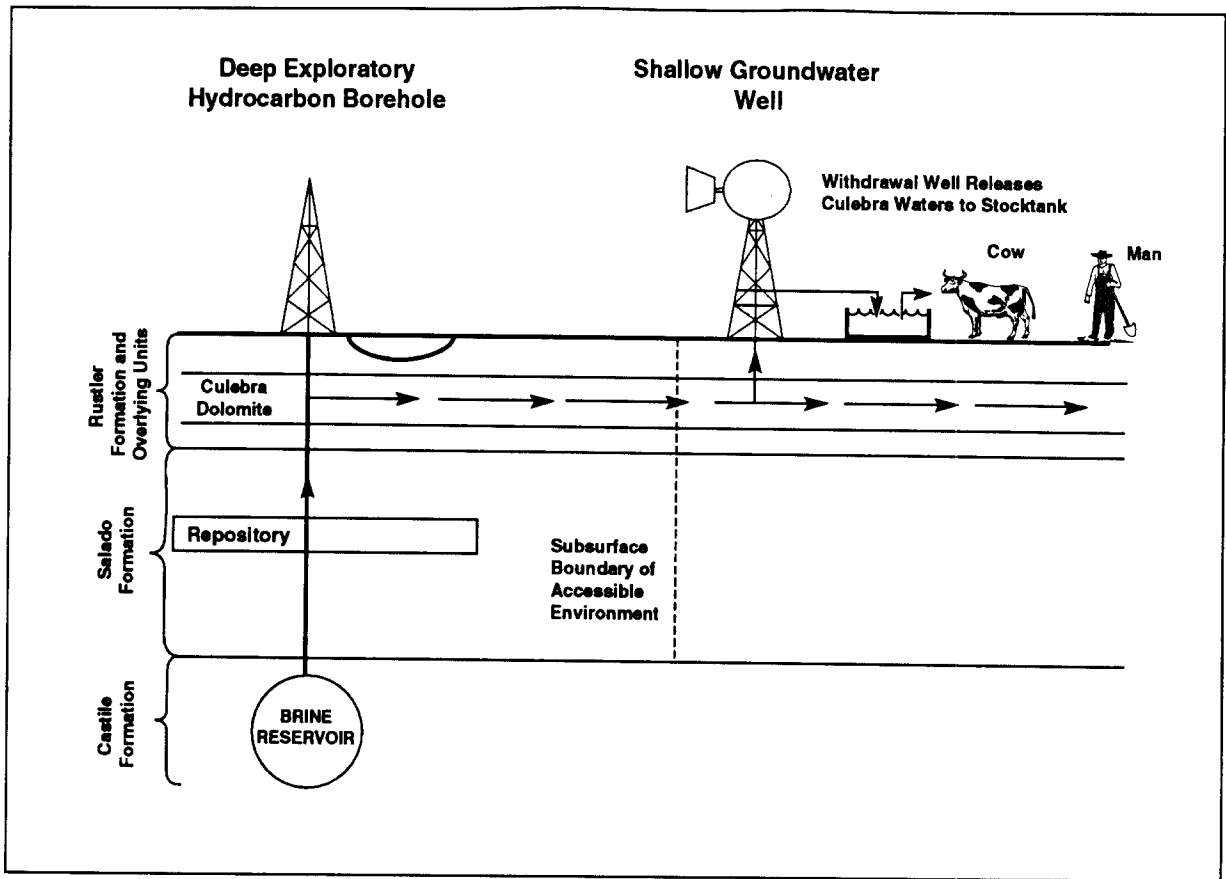


Figure 6 Radionuclide release scenario for the Level 2 exercise. The transport route of interest involves vertical flow through the repository to the Culebra Dolomite, horizontal transport through the Culebra to a point 5 km away, where release to the biosphere occurs via withdrawal from a shallow well.

transmissivity field were provided, even though different spatial distributions and configurations of aquifer transmissivity could be justified on the basis of the available data. In addition, the source term for radionuclide release into the aquifer, and a biosphere model, were provided.

Stage 2 of the exercise would involve consideration of multiple transmissivity fields consistent with the data. The impact of that uncertainty with uncertainties arising in Stage 1 modelling would be compared. In Stage 3, a wider range of conceptual model uncertainties would be addressed.

However, the decision to terminate the activities of the PSAG in 1994 meant that only Stage 1 of the Level 2 exercise could be carried out, and the remainder of this description is therefore restricted to Stage 1.

Participation in the Stage 1 exercise involved calculating groundwater flow in the Culebra aquifer on the basis of a given fixed transmissivity field and set of pressure-head boundary conditions (or optionally starting from a flow field pre-calculated by SNL), calculating

radionuclide transport within the aquifer using the conceptual model of the participant's choice, on the basis of a supplied source term, and calculating doses on the basis of the specified conceptual model. Input data for most model parameters were specified, either as fixed values or as PDFs, but the same database was used by all participants. No attempt was made to restrict the choice of conceptual model for radionuclide transport, apart from the requirement for consistency with the given data.

Participants were asked to compute cumulative releases of radioactivity at specified boundaries and at specified times up to 10,000 years, release rates, peak releases and peak doses, and the times of occurrence of the peaks.

The radionuclides whose transport was to be calculated were specified as the members of the single (simplified) decay chain: $^{234}\text{U} - ^{230}\text{Th} - ^{226}\text{Ra} - ^{210}\text{Pb}$.

The definition of conceptual model uncertainty

Although there was much interest in conceptual model uncertainty within the PSAG and in other quarters, there was, at the time of formulating the Level 2 exercise, no universal agreement regarding the definitions of 'conceptual model' or 'conceptual model uncertainty'. The following definitions were adopted by the PSAG for use in the Level 2 exercise:

Conceptual Model: A set of qualitative assumptions used to describe a system or subsystem for a given purpose. At a minimum, these assumptions concern the geometry and dimensionality of the system, initial and boundary conditions, time dependence, and the nature of the relevant physical and chemical processes. The assumptions must be consistent with one another and with existing information within the context of the given purpose.

Alternative Conceptual Models: Alternative sets of assumptions that describe the same system for the same purpose, where each set of assumptions is consistent with all existing system information.

Conceptual Model Uncertainty: The lack of knowledge about the system resulting from insufficient information to support or refute alternative conceptual models.

These definitions were communicated to the PAAG, and adopted as the working definitions for the NEA workshop on conceptual modelling uncertainty held in Paris in 1993 [NEA, 1995].

Two things are particularly worthy of note in the above definitions:

- First, conceptual model assumptions are not taken as being restricted to assumptions about the true nature of the system being modelled. For instance, according to this definition, groundwater flow in some region could be conceptualised as being two-dimensional, even though variations in the third dimension may exist. Other definition

schemes would be possible, such as classifying choices like dimensionality under a separate heading of numerical approximations.

- Second, the assumptions that comprise a conceptual model are 'for a given purpose'. Assumptions could be consistent with the existing information when they are to be used in modelling for one given purpose whereas the same assumptions could be inadmissible in the context of a different purpose. For instance, an assumption of constant conditions may be valid for the purpose of modelling behaviour for one thousand years, but inadmissible for the purpose of modelling for a million years.

Results of Level 2 Stage 1

Six organisations participated in the exercise. Some participants submitted more than one set of results, using different models for radionuclide transport. The most significant elements of difference between participants' choices of conceptual model for transport of radionuclides were dimensionality (one or two dimensions), whether fractures in the rock were explicitly taken into account, or an effective porous medium representation used, whether the transport was considered to be restricted to the fractures, or to involve diffusive transfers into and out of the rock matrix between the fractures, and whether retardation by sorption was included.

The problem specification called for several measures of performance to be evaluated. Those relating to a particular time were restricted to times up to 10,000 years. Peak release rates and doses, and times of peak, were called for, but comparisons were difficult because participants' calculations were terminated at different upper time limits. It was clear that the peak release rates at most boundaries were likely to occur long after 10,000 years when models were used that allowed access of radionuclides to the full porosity.

Some participants initially ran only a small number of sample cases in their PSA calculations – as few as 35. In analysing the results, it became evident that this was inadequate for consequence measures used in the exercise. Participants using one-dimensional models were able easily to provide many hundreds of sample runs, whereas the greater complexity of two-dimensional models made this difficult for some participants. No definite principle was found for determining an adequate sample size to obtain convergence for the mean of a given output quantity. It is clear that the required sample size for convergence depends on the output quantity concerned, and that simple rules of thumb, relating sample size to the number of model parameters, cannot have universal validity.

The results submitted by participants varied considerably - some by orders of magnitude - for all consequence measures (cumulative releases, release rates, doses). However, for many transport model conceptualisations, peak release rates and doses occurred later than 10,000 years, the time cut-off for this exercise, and release rates and doses were very small (or zero) in the initial 10,000 years. In such cases, intercomparison of results after only 10,000 years may overstate essential differences between models.

The feature of the different conceptual models contributing most strongly to the differences in results was judged to be the assumed amount of accessible porosity. The porosity contributed by the fractures in the rock is much smaller than the total including the rock matrix. Models that allowed for the radionuclides entering the matrix porosity, either through explicit representation or by use of a porous-medium model in which the assumed porosity value included the matrix contribution, gave much later releases to the more distant boundaries.

Other factors must also have contributed to the differences in the results, but the information supplied by the participants was insufficient to enable a full understanding to be obtained. The use of different numerical approximations is assumed to be a likely cause of most of the unexplained discrepancies.

Conclusions and lessons from Level 2 Stage 1

The exercise succeeded in assembling a variety of alternative model treatments for radionuclide transport, none of which were judged to be inconsistent with the information provided in the problem specification. In a real assessment exercise, it may be possible to assemble information that could limit the range of conceptual models to a much greater degree, and the context of the modelling might be more tightly prescribed. Indeed, were such a very wide range of results to be obtained from alternative conceptual models in a real assessment, it is likely that efforts to reduce the range of conceptual model uncertainty would have a high priority³.

The issue of alternative conceptual models being admissible in the context of a given purpose was highlighted by participants who employed fracture-only transport models, in order intentionally to give a conservative treatment of the uncertainties. As a result, very rapid releases were calculated. Such an approach was considered to be acceptable within the purpose of the exercise. However, it is difficult to address questions about the relative importance of conceptual modelling uncertainty and other sources of uncertainty if conservative and realistic modelling approaches are both to be considered equally admissible. If an arbitrary degree of conservatism is admitted, it is possible to arrive at an almost unlimited range of answers for many performance measures.

Complex exercises require significant resources to be committed by participating organisations. The earlier PSACOIN exercises could be done well by individual modellers working relatively independently. The level of complexity of exercises such as Level 2 is such as to require teams of participants, with a variety of expertise, covering several of the areas required for a national assessment. This aspect of the Level 2 exercise was partly

³ Indeed, later experimental work at the WIPP focused on achieving better understanding of the physical and chemical retardation properties of the Culebra.

responsible for the diminishing number of groups that were able to participate actively in the PSAG as Level 2 became the principal focus.

International modelling exercises always require more than one round of analysis and evaluation of results if they are to achieve a successful completion. The PSACOIN Level 2 exercise suffered in this regard from the termination of the PSAG's activities. The Level 2 Stage 1 results showed some features that could not be adequately explained. This provides a lesson, not only for the conduct of international code comparison exercises: performance assessments should be conducted iteratively, and they should receive external review, to help identify potential errors and important removable uncertainties in the assessment results.

6. Summary of Achievements of the PSAG

By sponsoring the existence and activities of the PSAG, the NEA has provided important and timely support for a number of OECD member countries in a period in which they were seeking to develop a capability to conduct safety assessments for potential and actual radioactive waste repositories. The whole process of developing concepts for the disposal of radioactive waste, identifying and evaluating potential disposal sites, and assessing the long-term radiological safety of specific repositories, has aroused strong interest from a variety of parties, and will continue to be subject to intense and searching scrutiny. In this context, most countries have seen as very valuable the search for international consensus with regard to philosophy and methodology, and the possibility to enhance confidence in their assessment tools by international co-operation and mutual review.

The major goals of the PSAG have been to promote the exchange of information, ideas and computational tools between participating organisations, and to help to build confidence in PSA methodology in general, and in the PSA codes used by participants in particular.

Information exchange

The effective exchange of information was encouraged by drawing together from many countries experts in a highly specialised field. The PSAG membership has always included many who were actively engaged in the development of PSA codes, and who were therefore intimately familiar with the practical details of implementing the PSA methodology. The discussions of the PSAG have thus always been strongly grounded in the practicalities of applying PSA. The PSAG was a group where a complex methodology was applied in practice, not simply talked about.

The PSAG has also benefited from a significant presence of those who were involved in shaping the direction of national programmes for assessing real waste disposal repositories. The Group therefore not only constituted a valuable source of first-hand information, but also influenced the formulation of national approaches to repository assessment. PSAG Member countries were at different stages in their development of safety assessment methodology and, for some groups, the PSAG was the starting point for their developments. Participation in the PSAG has come from more than ten OECD Member countries, as well as from the European

Commission and the International Atomic Energy Agency. The work of the PSAG has continually been reviewed by the NEA Performance Assessment Advisory Group.

The activities involving information exchange and technical discussion have covered wide ground, including the design of PSA codes, development of specific submodels for PSA codes, the theory of statistical convergence, the fundamental basis for treating uncertainty in probabilistic terms, reduction of research codes to practical assessment tools, sensitivity analysis, and elicitation of expert opinion.

Code intercomparisons

The goal of the PSAG to help build confidence in the computational tools used by Member groups in safety assessments was achieved principally through the PSACOIN intercomparison exercises. These were conducted in a series of 'Levels', designed first to test the basic framework of PSA codes, and then to move progressively towards greater realism, in the sense of studying test cases similar to real assessment problems, and in using models drawn from those actually being used in national programmes.

Levels 0 and E tested the executive functions of the participating PSA codes, including random generation of parameter values from specified probability distributions, and the statistical analysis of results. Practical attention to these questions brought to light the need to select effective ways of presenting PSA results, and the difficulties of giving precise meaning to the question of which model parameters are the most important.

Levels 1a and 1b represented deep and shallow disposal systems in a more realistic way, giving some freedom to participants to use submodels developed for use in their national programmes. These exercises, by raising the question of how wide a range of different models could validly be applied to a particular problem, led to Level 2, in which uncertainty associated with model choice began to be more fully examined. Level 1b also gave a valuable opportunity for members to gain experience in the incorporation of some complexity into the biosphere models used within a PSA calculation.

A general result of Levels 0, E, 1a and 1b was that the results from the different codes were substantially in agreement, where such agreement could be expected in the light of the models being used.

The Level S exercise specifically addressed methods for sensitivity analysis. It differed from the other PSACOIN exercises in concentrating more on methodology than on comparison of results obtained using different codes applied to the same problem. The published report contained articles contributed by participants, and some of these articles present new approaches and techniques for sensitivity analysis.

Finally, Level 2 represented a major increase in complexity and realism, attempting to address the question of the relative importance of parameter-value uncertainty and

uncertainty with regard to choice of conceptual and mathematical models where alternatives exist that cannot be ruled out on the basis of available information.

Final status

At the time of the final PSAG meeting, key technical issues in PSA had been discussed and documented by the Group, and five code intercomparison exercises and a Brochure on PSA had been published. The Level 2 exercise was still incomplete (and thus has not been published). Further international attention to these matters may be achieved in the future through other means. At this stage, many of the national groups that participated in the PSAG are actively engaged in preparing or defending safety cases for proposed repository developments, or in the use of PSA methods to underpin the regulatory evaluation of such safety cases. Others are continuing in the process of justifying disposal concepts and examining alternative disposal sites. The work of the PSAG has created a set of reports on technical issues that will continue to be relevant to these activities, and the published PSACOIN exercise results provide a set of benchmark tests that can be used as part of the verification of new PSA codes.

7. Issues Deserving Further Attention

The PSAG has had a decade of fruitful work. The Group's remit was not to answer completely all questions regarding PSA and its application to radioactive waste disposal, and it has not done so. The way forward for international co-operation in this technical area is not yet clear. This Chapter provides a brief account of some of the issues that may be worthy of further international work.

7.1 Issues in the Fundamentals of the Treatment of Uncertainty

The validity and merits of the probabilistic approach

Most countries involved in the use of nuclear power have established regulatory guidelines for the evaluation of schemes for disposal of radioactive wastes. However, few regulatory frameworks are explicit about the nature of uncertainty, what language is appropriate to discuss it, and the way in which uncertainty should be taken into account in assessments.

The work of the PSAG has been based on probabilistic approaches to treating uncertainty, under the assumption that the theory of probability provides an appropriate basis for quantifying uncertainties and for combining uncertainties. Nevertheless, the PSAG has been open to the debate on the relative merits of other approaches to treatment of uncertainty, and Fuzzy Set theory in particular has been discussed (see Chapter 4). One issue discussed by the PSAG concerns the appropriateness of using probabilistic language when eliciting expert judgements about parameter values when there is a marked lack of direct experimental evidence. Thus, the PSAG has also debated the idea that different types of uncertainty should be distinguished, and handled differently. The PSAG did not reach definitive views in any of these debates.

Some countries are not currently using PSA in preparing assessments for proposed waste repositories. Rather, deterministic analyses are made, often using a combination of 'best-estimates' and conservatism as the means of dealing with uncertainty. A conservative analysis deliberately selects models and parameter values in a way that should tend to overestimate risks or other similar performance measures. An advantage of such approaches is that results can be easier to communicate and understand.

On the other hand, models in some PSA codes have a tendency to be simpler than in purely deterministic approaches since a large number of computer runs have to be performed. The use of generally simpler models in PSA may require conservative assumptions to be made within the analysis.

The use of conservative approaches, whether within a purely deterministic framework or as part of a PSA, is respectable, but open to some concerns. For example, in a system with many components and many sources of uncertainties, many conservative assumptions may have to be made. In combination, they may lead to prediction of unacceptable system performance, whereas an assessment that was realistic at every turn may well have predicted acceptable performance. Furthermore, the calculated impacts may poorly represent the expected performance of the disposal system, making the model results poorly suited as a basis for optimising design, focusing data collection programmes, or improving the safety and cost-effectiveness of the disposal system.

In attempting to move away from conservatism, a strength of the PSA approach is that, in principle, it allows all uncertainties that can be characterised by probabilities to be considered within a coherent, unified framework, and ensures systematic searching of all combinations of parameter values.

Further consideration at international level on the relative merits and roles of deterministic and probabilistic assessment approaches within a safety case would be valuable.

Can PSA only handle some types of uncertainty?

It is sometimes asserted that PSA is a tool for dealing with one type of uncertainty, that associated with the values of model parameters, whereas other types of uncertainty, such as uncertainty in model structure, cannot be dealt with using PSA. This assertion is open to debate, and it is a matter still to be determined exactly which types of uncertainty can, or should, be treated in this way.

One thing is certain: if an aspect of uncertainty about the system being studied cannot be quantified in probabilistic terms, it cannot be treated by a probabilistic assessment method. For instance, in any assessment, it is possible that human errors have been made in assembling the data, in reporting the results, or in the writing of the computer code. But it appears to be impossible to assign a probability distribution to the magnitude of any such undetected errors, so it is impossible to deduce a quantitative estimate of the impact of such outright errors on an assessment result.

It is more difficult to decide about the applicability of PSA to the class of uncertainty associated with the possibility of using several alternative models to represent the same phenomena. Conceptual model uncertainty (CMU) was at the centre of the concerns of the PSACOIN Level 2 exercise, but that exercise was not able to draw firm conclusions about the relative importance of CMU and other classes of uncertainty, nor about the amenability of

CMU to treatment within the framework of a PSA calculation. CMU was also the subject of a recent NEA Workshop [NEA, 1995], but again, the question of the applicability of PSA was not settled.

Sometimes, the existence of a range of applicable models, none of which can be ruled out by the available evidence, can be represented in parametric terms. For instance, for transport of radionuclides by groundwater flowing in a fractured rock, there may be uncertainty as to whether the rock matrix between the fractures is accessible to the radionuclides, giving the possibility of greatly retarding their transport. A model that includes diffusion into the rock matrix and a model based on transport only in the fractures may be considered as alternative models, with some uncertainty as to which is applicable in a particular medium. However, it is perfectly possible to construct a model that represents both fracture transport and rock-matrix diffusion, including one or more parameters that affect the ease of access of solutes from the fractures into the matrix. Assigning PDFs to these parameters could have a similar effect to attributing probabilities to the two alternative models. Thus, one outlook, in which the analysis was treated as a single model with parameter uncertainty, could be considered equivalent to another outlook, in which conceptual model uncertainty was said to exist.

In summary, PSA is capable, from a computational point of view, of handling any type of uncertainty that can be characterised by probabilities. Casting uncertainties in parametric form is straightforward: even choices between apparently unrelated alternative representations can be cast mathematically in terms of a discrete probability distribution for an integer that selects between the alternatives. The difficulty lies in attributing the probability distributions in a way that is defensible.

Risk dilution

In assigning PDFs to describe the uncertainty in the parameters in a PSA, there may be a tendency to overestimate the uncertainty, that is, to overestimate the width of the parameter distributions. The term 'risk dilution' is used to describe a situation in which an increase in the uncertainty of the input parameters of a model (while holding the mean of the distributions constant) leads to a decrease in the mean of an output quantity. While this output quantity may be a risk, the concept could also apply to other possible performance measures. If overestimation of uncertainty results in mean consequences being reduced, the unfortunate effect is that what appears to be a conservative step (overstating the degree of uncertainty) leads to an overoptimistic assessment of mean system performance.

One circumstance in which risk dilution is a concern is when the performance measure in question (for instance individual dose rate) has a peak in time, and the time of the peak is affected by one or more of the uncertain parameters. Averaging over the possible values of the model inputs amounts to averaging over alternative situations in which the peak value of the performance measure occurs at different times. At any given time, the mean value of the performance measure is obtained by averaging cases that lead to the peak occurring at around

that time with others for which the consequence is relatively small. Clearly, the mean value is less than the maximum value at any given time. The wider the distribution of the parameters, the wider the range of peak times, and the more the averaging process mixes in relatively small values. Hence the term 'dilution'.

Guarding against unwarranted risk dilution is part of the process of developing PDFs for radioactive waste disposal PSAs. It would be of interest to reconsider the potential importance of risk dilution as an issue in PSA if decisions were based on measures of system performance other than 'mean' values (for example, particular percentile values could be used as an alternative).

Time dependence and other model complexities

All the model systems studied in PSACOIN exercises calculated outputs that were functions of time. However, the nature of the mathematical models was unchanging with time, and the boundary conditions were constant. The same is true of the majority of practical applications of PSA to waste repository safety that have been performed around the world to date. The work of HMIP in the UK is an exception in this regard, providing the first full-scale demonstrations of performance assessment in which probabilistic techniques have been used to simulate time-varying boundary conditions [e.g., Sumerling (Ed.), 1992].

The desire for accuracy tends to imply that known time-dependent aspects of the system that could have a significant effect on calculated system performance should be represented in the model. However, models with time-dependent boundary conditions are harder to implement than those with constant ones, and the problem of specifying parameter distributions when the parameters can be general functions of time deserves more study. In the face of such difficulties, some argue that explicit treatment of time dependence should be avoided if possible.

Closely related to the question of how time dependency is treated in PSA is the methodology used for forming and defining 'scenarios' for consequence analysis. There has been a good deal of discussion within the PSAG and elsewhere concerning the relative benefits of an all-embracing approach to system simulation versus the development and representation of a relatively small number of scenarios to describe the future evolution of the disposal system. In both approaches, all features, events and processes (FEPs) of concern are identified. In system simulation, as advocated most forcefully by HMIP in the UK, all such FEPs are combined into an overall model of the evolving disposal system and its environment. Probabilistic techniques are used to account for FEPs of uncertain occurrence or timing that cannot be explicitly modelled. For example, in the HMIP demonstration of this approach, changes in groundwater flow resulting from climate change are explicitly modelled, although the changes in climate are accounted for probabilistically. In the scenario approach, one or more potentially disruptive FEPs is explicitly kept outside the main 'base case' assessment model. Typically, these FEPs are of uncertain occurrence or timing, and their consequence is

assessed by hypothesising and modelling a series of discrete futures. Relations between these scenario-forming events and processes are not always explicitly considered; rather, each discrete future may be assigned a 'weight' for the purpose of combining overall results (e.g., into CCDFs).

There is often confusion about the essential differences between scenario-based and simulation-based approaches. The distinction between the two approaches is increasingly seen as more terminological than real. All scenario-based approaches rely on simulations of disposal system performance using calculational models. The environmental simulation approach, as advocated by HMIP, can be considered a variant of the scenario approach, in which several additional events and processes - that is, those associated with natural climate change - are coupled in an overall system assessment model. Whether the scenario or the simulation approach is used, the objective is to produce a model of long-term system behaviour. In both approaches, a complete conceptual model of the system is developed and, in practice, subjective judgements, scoping calculations, and available computational capabilities are used to decide which processes and interactions should be included in system-level consequence analyses.

In principle, given access to the same information base and the same experts, the results of a scenario-based approach should be comparable to those from a simulation model. Limited attempts at comparison of the two approaches have been made within PSA [e.g., Sumerling (Ed.), 1992], but a convincing argument that use of the two approaches would lead to fundamentally different assessment conclusions is yet to be made. The question of when it is necessary to model time-dependencies explicitly, when they can be ignored, and when time-invariant scenarios can be used as a substitute, will need to be addressed in the context of the purpose and requirements of particular national assessments. However, further work at international level may help to inform the response (see next section).

As proposed repository sites are studied, increasing levels of site-specific information are becoming available. Furthermore, computer power is continuing to increase, giving the possibility of using more and more complex models as part of PSA calculations. This applies not only to incorporation of time-dependent effects, but also to the treatment of spatial variation, possibly in three dimensions, in flow and transport submodels. Some within the PSAG have questioned whether this trend would necessarily represent a real gain. Will it increase confidence in the results, or rather tend to obscure the dominant features of the system on which safety relies? Is it possible that the incorporation of more detail, with the concomitant need to specify more parameters, could lead to an increase in the overall uncertainty in the calculated performance measures? If so, is this appropriate? Again, although such questions will need to be addressed in the context of the purpose and requirements of particular national assessments, further work at international level could help inform the response.

7.2 Issues in PSA Methodology

Convergence

The issue of the convergence of PSA results was referred to briefly in the discussion of statistical sampling schemes in Chapter 4. This issue is distinct from the more general issue of numerical convergence, which is relevant to all numerical modelling, whether conducted deterministically or within a Monte Carlo framework. Convergence of PSA results is an important issue because the results produced by an application of PSA must be reliable, yet the method by its nature involves repeated calculations using numerical models, and these can consume much computer time, the more so as the models are made more realistic. In many applications of PSA to date, the sample sizes used have been determined mostly by intuition, operating within constraints of expense, or elapsed time, associated with computer execution time.

Achieving convergence, and having confidence in the fact, may be more difficult in PSA applied to waste disposal systems than in many other applications of Monte Carlo simulation, because of the skewed distributions of output values that seem to arise. If, for instance, a value that is at least 100 times bigger than the mean occurs with a probability of 1 in 1000, a sample size of 100 cases would have only one chance in ten of encountering such an extreme value. Yet if such an extreme value did arise, it would contribute to the estimated mean at least ten times more strongly than it should. The accuracy of the mean estimation would thus be very poor with a sample size of 100; a sample size of several thousand would be more appropriate.

In the PSACOIN Level E exercise, a scheme for testing convergence was examined, based on dividing the sample results up into batches, and looking at the distribution of the means of the batches. The results obtained in this exercise gave no grounds for believing in the efficacy of this test scheme.

The PSA method makes it possible to accompany estimates of means or other statistics with a measure of the estimation accuracy. However, such error analysis is based on the variability observed in the sample cases that were examined, and there is always some doubt that the error estimate may be smaller than is really justified. To be assured of convergence, some information about the shape of the consequence distribution is required, independent of the evidence provided empirically by the samples taken so far. Automatic 'stopping rules' should therefore be viewed with caution.

It is likely that the number of sample cases required for convergence and for attaining a given estimation accuracy depend on the nature of the output quantity. For instance, the cumulative release to the surface of a parent radionuclide cannot possibly exceed the disposed inventory. There is therefore no question of the upper tail of the distribution extending beyond this limit. For this reason, the mean of a cumulative release may converge much more rapidly than, say, the mean release rate at a certain time. It appears, however, that no systematic studies have

yet been made on the relationship between convergence and the choice of performance measure.

Convergence is also an issue for sensitivity analysis. A conclusion of the PSACOIN Level S exercise was that, for a given number of samples, measures of parameter sensitivity can be much further from convergence than the means calculated as part of uncertainty analysis. This is because parameter sensitivities are likely to depend significantly on the precise shape of the output distribution, and this, therefore, may need to be shown to have converged statistically in order to have confidence in measures of parameter sensitivity.

Parameter correlation

The question of correlation among the uncertain parameters of a model to which PSA is applied has only briefly been considered by the PSAG. The matters requiring attention lie in two areas. First, it is difficult to communicate the meaning of correlation where subjective uncertainty is concerned. In the case of two or more stochastic quantities that may be sampled by repeated observations, the joint probability distribution may be interpreted in frequentist terms. If the observation of a large value for one variable is frequently accompanied by the observation of a large value for another variable, the two can be said to have a positive correlation. However, for most of the uncertain parameters of models of the long-term performance of waste disposal systems, there is no question of repeated observations, although some of the parameters may relate to quantities, such as rock properties, that in principle could be measured at different locations or times. Rather, the PDF attributed to each parameter represents a degree of belief on the part of experts (conditioned perhaps by experimental observations of measurable quantities) in the appropriateness of using different values of that parameter in the assessment. Correlation between two parameters then has to be expressed in terms such as the following: “A positive correlation could be said to exist if experts believed that the revision of one parameter’s value, to lie at the high end of that parameter’s PDF, would result in the value of a second parameter being revised upwards.”

The second issue concerning parameter correlation is that of specifying the correlation quantitatively, and implementing the correlation in the Monte Carlo sampling. It may appear to be easy to elicit an expert judgement of the correlation coefficient applying between two parameters, but simply specifying the correlation coefficient is insufficient in general to specify the full joint PDF, which gives the probability density in the neighbourhood of any given pair of values.⁴ Discussions on this subject within the PSAG have revealed that some members have tried a scheme in which tables of sampled parameter values have their entries permuted at random, until the correlation coefficients reach the required values. However,

⁴ Multivariate Normal distributions provide a special case in which correlation coefficients suffice to specify the full details of the covariation.

this is a somewhat arbitrary, and generally non-unique, basis for achieving the required degree of correlation.

It would appear preferable, when possible, to discover the physical basis for belief in a correlation between two parameters. Usually, it means that they both depend on another set of variables, involved in the fundamental processes underlying the meaning of the parameters. If those underlying variables can reasonably be attributed independent (uncorrelated) distributions, and if analytic expressions can be stated relating these independent variables to the model parameters, then those parameters will become dependent random quantities that in general will be correlated.

Types of system model

The model systems studied in the PSACOIN exercises, and much of the experience of applying PSA that has been discussed by PSAG members, have been concerned with the groundwater pathway for transport of radionuclides from a repository to the accessible environment. A notable exception is the work of SNL in the US for the WIPP, which has considered both two-phase flow and human intrusion releases [WIPP PA Division 1991; WIPP PA Department, 1992]. On the basis of the SNL work, there do not appear to be particular problems associated with applying PSA to models of other major pathways, but the PSAG did not as a Group explore the treatment of alternative release pathways in PSA. For example, it is possible that convergence for PSA applied to human intrusion events may be harder to obtain than for PSAs that consider groundwater releases alone. This is because the human intrusion pathway may be dominated by the effects of intrusion events that are relatively short-lived, and occur at unpredictable intervals, whereas groundwater-mediated transport gives rise to long-lasting releases, for which uncertainty in the parameters results in relatively minor variations in timing and magnitude of the consequences.

7.3 Issues in the Application of PSA

Visualisation of model results in the presence of uncertainty

The concept of uncertainty is difficult to communicate, especially when the quantities calculated are functions of space and time. Communication of assessment results is an issue no matter what assessment approach is adopted. However, the issue is made more difficult when statistical concepts need to be communicated to a broad audience. PSAG members have expressed the view that further advances in the art of communicating such results must be possible but, although discussed, this has not been a focus of work within the Group.

Termination of the data-gathering/assessment cycle

Typically, PSA is applied as part of an iterative process of site characterisation and performance assessment. For example, an initial characterisation of a proposed disposal site

may be followed by a preliminary PSA. Further research and data collection may follow, aimed at providing less uncertain values for model parameters, and providing greater confidence in the choice of models and in the understanding of the site. Using the information thus gathered, a refined assessment will be carried out. However, this cycle could continue indefinitely, in a continual drive to reduce remaining uncertainties. Although reduced uncertainty may always be desirable, there remains the need to identify the point at which sufficient assurance exists that decisions can be taken to permit construction of the waste repository, emplacement of waste and, finally, repository closure.

The PSA method can be used to help close out the decision process described above in two ways. First, as discussed in Chapter 2, a PSA result such as a mean dose can be provided with associated measures of estimation uncertainty, such as 95% confidence limits. These measures help to ensure that uncertainty associated with the Monte Carlo sampling itself is not dominating the overall uncertainty in the PSA. Second, as discussed in Section 5.5, sensitivity analysis can help identify the model parameters whose uncertainty most contributes to the uncertainty in the calculated system performance, and can quantify the potential reduction in overall uncertainty if the model parameters were better characterised. Similar kinds of analysis can be brought to bear regarding uncertainties over the choice of conceptual or mathematical models.

Closure of the decision process becomes clearer where decision makers can agree standards in advance specifying the degree of remaining uncertainty that is acceptable at any stage of the decision process. This does not appear to be difficult in principle, and forms an integral part of regulations in some countries [e.g., US EPA, 1993; 1996]. More troublesome for the decision process may be the existence of uncertainties that are difficult to quantify, such as the concern that the analysts have not accounted in the PSA for some potentially important site-specific feature, event or process.

7.4 Recommendations

The NEA could usefully follow up the PSAG work that has been described by focusing on issues mentioned in this Chapter. Also, more recent developments in PSA could be examined. The issues highlighted here include:

- How to ensure understanding of the process of PSA, and of its results by the various stakeholders in the decision process.
- How to ensure traceability of information flow throughout the assessment process.
- The treatment of conceptual model uncertainty, and whether it is generally reducible to parametric uncertainty.
- The treatment of time dependency in PSA.

- The treatment of correlated input parameters.
- Statistical convergence, and sensitivity analysis.
- Re-evaluation of the issue of risk dilution in light of evolving regulatory considerations on the definition of risk.

The emphasis within the PSAG was on the development and application of tools and techniques for the estimation of radiological performance under uncertainty, regardless of the purpose of such analyses. However, a regulator and a proponent will perform PSAs for fundamentally different reasons. For example, a proponent may conduct a PSA to support a safety case on repository development, and a regulator may use PSA independently to help evaluate such a case. The question of how best to employ PSA in the context of regulatory review may become an increasingly important issue as more repository safety cases that incorporate PSA are submitted for formal regulatory review.

PSA as such should not be regarded as an activity that is purely code related, and concerned only with simple models. Rather, it has been used by PSAG members to encourage a comprehensive and traceable account of assumptions and decisions made in the presence of uncertainty at all stages of preparation of a safety case (and its corresponding regulatory review), whether or not a simplified computational model is derived. The NEA has already encouraged new initiatives focusing on the entire procedure of building a safety case, from collection, collation and interpretation of data, through detailed modelling and bounding estimates of performance, through full Monte Carlo simulation where considered necessary, and further work devoting to clarifying the relationship between the use of ‘deterministic’ and ‘probabilistic’ modelling approaches would be desirable.

Finally, international exercises to compare realistic approaches to performance assessment, as proposed originally for the PSACOIN Level 2 exercise, may require resources and commitment on a scale approaching that of a real assessment. The effect of differing amounts of site information on the performance estimate is a key concern in view of the very large resources involved in such investigations and the subsequent interpretation of the data. One purpose of the PSACOIN Level 2 exercise was to examine this problem. The Level 2 specification could be usefully re-examined to see if a new international exercise could be of mutual benefit.

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