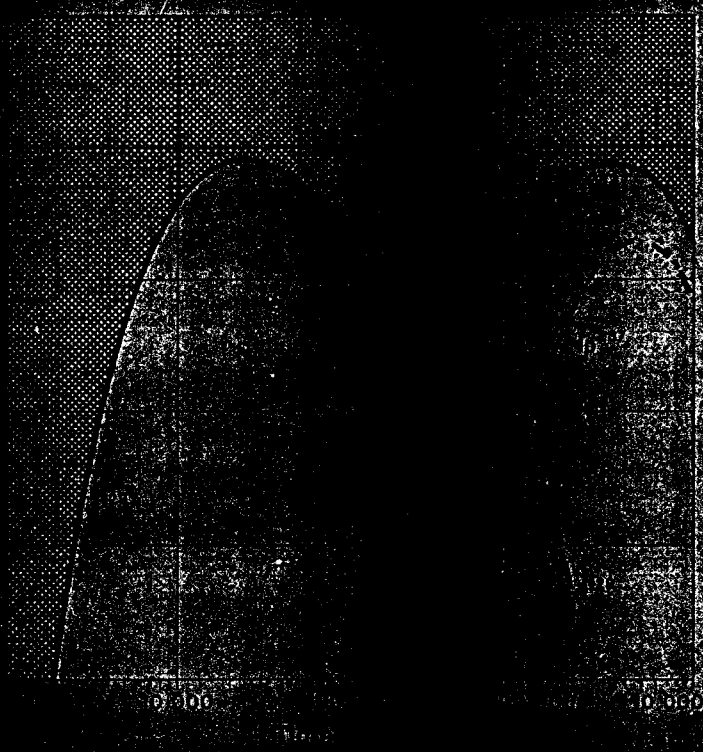
An International Code Intercomparison Exercise on a Hypothetical Safety Assessment Case Study for Radioactive Waste Disposal Systems

PSACOIN LEVEL E INTERCOMPARISON

Probabilistic System Assessment Code (PSAC) User Group



NUCLEAR ENERGY AGENCY

OCDE
OECD

PARIS 1989

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NUCLEAR ENERGY AGENCY
ORGANISATION FOR ECONOMIC CO-OPERATION AND DEVELOPMENT

Pursuant to article 1 of the Convention signed in Paris on 14th December 1960, and which came into force on 30th September 1961, the Organisation for Economic Co-operation and Development (OECD) shall promote policies designed:

- to achieve the highest sustainable economic growth and employment and a rising standard of living in Member countries, while maintaining financial stability, and thus to contribute to the development of the world economy;
- to contribute to sound economic expansion in Member as well as non-member countries in the process of economic development; and
- to contribute to the expansion of world trade on a multilateral, non-discriminatory basis in accordance with international obligations.

The original Member countries of the OECD are Austria, Belgium, Canada, Denmark, France, the Federal Republic of Germany, Greece, Iceland, Ireland, Italy, Luxembourg, the Netherlands, Norway, Portugal, Spain, Sweden, Switzerland, Turkey, the United Kingdom and the United States. The following countries became Members subsequently through accession at the dates indicated hereafter: Japan (28th April 1964), Finland (28th January 1969), Australia (7th June 1971) and New Zealand (29th May 1973).

The Socialist Federal Republic of Yugoslavia takes part in some of the work of the OECD (agreement of 28th October 1961).

The OECD Nuclear Energy Agency (NEA) was established on 1st February 1958 under the name of the OEEC European Nuclear Energy Agency. It received its present designation on 20th April 1972, when Japan became its first non-European full Member. NEA membership today consists of all European Member countries of OECD as well as Australia, Canada, Japan and the United States. The commission of the European Communities takes part in the work of the Agency.

The primary objective of NEA is to promote co-operation among the governments of its participating countries in furthering the development of nuclear power as a safe, environmentally acceptable and economic energy source.

This is achieved by:

- *encouraging harmonisation of national regulatory policies and practices, with particular reference to the safety of nuclear installations, protection of man against ionising radiation and preservation of the environment, radioactive waste management, and nuclear third party liability and insurance;*
- *assessing the contribution of nuclear power to the overall energy supply by keeping under review the technical and economic aspects of nuclear power growth and forecasting demand and supply for the different phases of the nuclear fuel cycle;*
- *developing exchanges of scientific and technical information particularly through participation in common services;*
- *setting up international research and development programmes and joint undertakings.*

In these and related tasks, NEA works in close collaboration with the International Atomic Energy Agency in Vienna, with which it has concluded a Co-operation Agreement, as well as with other international organisations in the nuclear field.

Preface

The NEA Radioactive Waste Management Committee (RWMC) is an international committee of senior governmental experts familiar with the scientific, technological, and environmental issues involved in radioactive waste management. Established in 1975 and working in close co-operation with the NEA Committee on Radiation Protection and Public Health, the RWMC draws on the best expertise to review developments in the technologies of radioactive waste treatment, storage, and disposal, and to supervise the NEA programme in this field. One of its objectives is to improve the general level of understanding of waste management issues and strategies, particularly with regard to waste disposal, and to disseminate the relevant information.

The NEA Probabilistic System Assessment Code (PSAC) User Group was established by the Radioactive Waste Management Committee in January 1985 to help co-ordinate the development of probabilistic safety assessment codes in Member countries. It meets twice a year to discuss topical issues and code intercomparisons and to exchange information.

The NEA Data Bank undertakes the collection, validation, and dissemination of computer programs and scientific and technical data within the NEA's field of interest. It receives advice from a management committee representative of the participating countries, and among its tasks is the provision of scientific and computing support for radioactive waste management activities. The NEA Data Bank contributes to the work of the NEA Secretariat for the PSAC User Group, and provides facilities for code exchange and the analysis of code intercomparisons.

Abstract

The PSACOIN Level E exercise is the second in a series of planned code intercomparisons being conducted by the Probabilistic System Assessment Code (PSAC) User Group of the OECD Nuclear Energy Agency. This exercise includes intercomparisons of both deterministic and stochastic results between ten different codes developed for the probabilistic safety assessment (PSA) of radioactive waste repository systems, as well as comparisons with an "exact" analytical solution. For both deterministic and stochastic runs of the PSA codes, the analysis shows that most participating codes produce results statistically consistent with one another and with the exact solution. Thus, the executive portions of almost all participating codes appear to be functioning as intended. In addition, a contribution has been made to the verification of models that may eventually be used in formal assessments of radioactive waste disposal concepts or sites. Finally, this exercise was largely unable to demonstrate significant differences in efficiency between the different parameter sampling schemes used by the participants. It was found, however, that confidence intervals for estimated mean values based on Chebyshev's Inequality were reliably conservative, whereas so-called "normal" confidence intervals, as supported by the Shapiro-Wilk test, proved less reliable.

CONTENTS

Annexes

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This report includes case studies from each of the individuals listed above. The conclusions and recommendations presented here represent those of the PSAC User Group only, and do not necessarily express the views of any Member country or international organisation.

EXECUTIVE SUMMARY

The Probabilistic System Assessment Code (PSAC) User Group was established by the Nuclear Energy Agency in 1985 to assist in the development of probabilistic safety assessment (PSA) codes by Member countries of the OECD. PSA codes are used in the preparation of environmental assessments to help quantify the variability and uncertainty associated with the predictive calculations upon which such assessments may be largely based. In particular, PSA codes are of special interest in assessing concepts for the underground disposal of radioactive wastes.

A major goal of the PSAC User Group is to enhance confidence in the capabilities of PSA and associated codes. Code intercomparisons can provide evidence that different codes developed and operated by different groups produce similar results when applied to the same problem. Such evidence contributes to the verification of the codes involved.

This report documents the Level E intercomparison, the second in a series planned by the Group. There were four objectives for the Level E intercomparison:

(1) to verify the consistent operation of PSA codes and their associated postprocessing codes, by code intercomparison,

(2) to verify further the correct operation of PSA codes, by comparison with an analytical exact solution of the specified system model,

(3) to provide a basis for evaluating the relative efficiency of different parameter sampling schemes for stochastic analyses by examining confidence intervals on estimated mean values, and

(4) to conduct a case study using models that may eventually be used in formal safety assessments of radioactive waste disposal concepts or sites, and thereby contribute to the verification of these models.

Although the first of these objectives closely parallels an objective of the Level 0 intercomparison (NEA PSAC User Group, 1987), the second objective is unique to Level E, and is made possible on the basis of an analytical "exact" solution for the Level E system model (see Robinson and Hodgkinson, 1987). The exact solution corresponds to using an infinite sample size and, therefore, provides a "converged" mean risk for comparison with the stochastic output of PSA codes. The third objective was attempted as part of the Level 0 exercise, but a more systematic study was deemed desirable. The fourth objective was defined in order to gain experience with an overall system model incorporating specific submodels that might be used in formal assessment studies.

The degree to which these objectives have been met can be summarised as follows.

(1) The results from the 10 participating codes show a high degree of consistency for both deterministic and stochastic analyses, despite the use of different codes, sampling schemes, and sampling sizes. Such agreement contributes to the verification of the executive portion of PSA codes, as well as those submodels that might eventually be used in formal safety assessment studies.

(2) Results from most of the PSA codes also agree well with the exact solution. In one situation, a tendency was found for the PSA codes to agree better with each other than with the exact solution - specifically, there was a tendency to underestimate mean dose. This situation is thought likely to arise only at early times when the mean dose is far below its peak value. In principle, this problem can be avoided by taking larger sample sizes.

(3a) The exercise was unable to demonstrate any difference in efficiency between Latin Hypercube Sampling (LHS) and Monte Carlo (MC) sampling with regard to convergence of sample means. Further research is required to evaluate the relative efficiencies of the two methods in PSA applications typical for radioactive waste disposal systems.

(3b) Only one participant employed the Importance Sampling strategy. Because of the design of the Level E case, however, the value of this strategy was inadequately tested. A more complex case is required to evaluate the relative efficiencies of the two methods.

(3c) An additional conclusion is that confidence intervals based on Chebyshev's Inequality are reliably conservative, whereas the so-called "normal" confidence intervals, as supported by the Shapiro-Wilk test, are less reliable. The latter confidence intervals were shown in practice to be frequently too narrow - particularly with small sample sizes - based on a comparison of these intervals with the exact solution. An improved method for providing distribution-free confidence intervals, however, using Guttman's Inequality, has recently been discovered (Woo, 1989).

(4) The source-term and geosphere components of the system model are similar to submodels currently in use by many of the participants and may eventually be used in formal safety assessment studies by some of these participants. The Level E exercise has substantially contributed to the verification of the code for these submodels.

In summary, the Level E intercomparison exercise has made a substantial contribution to the verification of the participants' codes. It is recommended that further code intercomparisons be pursued, with greater emphasis on the use of system models that are more representative of specific concepts for the disposal of radioactive waste.

1. GENERAL INTRODUCTION

The Probabilistic System Assessment Code (PSAC) User Group was established in 1985 by the Nuclear Energy Agency (NEA) of the Organisation for Economic Co-operation and Development (OECD). The principal purpose of this Group is to further the development in OECD Member countries of computer codes for the probabilistic safety assessment (PSA) of radioactive waste disposal systems. Activities of the Group comprise information exchange, peer review, joint code development, discussion of topical issues, and code comparisons. The last activity is particularly important as formal code comparisons help to verify that codes developed for safety assessments are functioning as intended. PSA codes consist of "executive" functions, such as a sampling algorithm to select parameter values, and a set of numerical submodels that represent the system to be analysed. Statistical "postprocessing" codes are used in close conjunction with PSA codes. Code verification is viewed as a necessary first step in building confidence in the ability of PSA codes to provide meaningful information for safety assessments.

This report summarises the results and recommendations arising from the Group's second PSA code intercomparion (PSACOIN) exercise, known as Level E because of the existence of an exact analytic solution. It is the direct successor to Level 0 (NEA PSAC User Group, 1987). The existence of an exact solution in the Level E study is particularly important because it allows not only intercomparison between codes, but also a benchmark against which all codes can be compared. Other PSACOIN studies in progress include Level 1a, which incorporates a more realistic system model representative of deep geological disposal concepts.

1.1 Purpose of the Level E Intercomparison Exercise

The Level E intercomparison exercise was meant to fulfil four principal objectives.

(1) The exercise should verify the consistent operation of PSA codes and their associated postprocessing codes, by intercomparison of the results of different codes. For the PSA codes, this would address mainly executive functions, including input, output, internal data transfers, the implementation and linking of submodels, random-number generation, and sampling algorithms. For the postprocessing codes, the exercise involves intercomparison of the statistical analyses - in particular, means, standard deviations, and confidence bounds - necessary for stochastic calculations. This objective parallels the main objective of the Level 0 exercise (NEA PSAC User Group, 1987).

(2) The exercise should further verify the correct operation of PSA codes, by comparison with an exact solution of the specified system model. The exact solution available covers not only cases

where all model parameters are fixed ("deterministic runs"), but also cases where some model parameters are uncertain and are defined using probability density functions ("stochastic runs"). In the deterministic runs, the exact solution provides an "exact" value of dose as a function of time. In the stochastic runs, the exact solution provides a precise expectation value of dose as a function of time. By including both deterministic and stochastic cases, it should be possible to separate the effects of numerical inaccuracies in the model implementations from the statistical variations to be expected from the use of independent sets of sampled model parameter values.

(3) The exercise should provide a basis for evaluating different parameter sampling schemes for stochastic analyses. The attributes to be tested include rate of convergence of mean values for different sampling strategies as sample size is increased. Simple Monte Carlo (MC) sampling and Latin Hypercube Sampling (LHS) are both widely used with PSA codes. Importance Sampling (IS) has also been investigated; this, like LHS, is designed to produce more rapid convergence than MC for estimated means as the sample size increases. In addition, a related issue was examined: the reliability of two methods (Chebyshev and Shapiro-Wilk) for calculating confidence intervals on estimated mean values.

(4) The exercise should use a system model sufficiently close to practical assessment requirements for some production submodels to be used, rather than special code modules written for the purpose of the exercise. In Level E, the equations for the geosphere correspond to a physically plausible system, although the biosphere model in particular is still rather idealised and artificial. It was therefore considered that most participants' codes could use existing submodels for the release and transport of radionuclides; to the extent that such submodels could be used, the exercise would clearly be more valuable to the verification of the participants' code. It was also recognised, however, that most participants' codes would require modification or extension to enable the case specification to be adequately represented. Some codes also required modification to be able to provide results in the form requested.

It was also initially considered that sensitivity analysis of the Level E output should be performed with the purpose of intercomparing the results of various possible analysis techniques. For reasons of clarity and timing, however, sensitivity analysis studies are limited to a ranking of radionuclides according to their contribution to mean dose. Other results may be published as a separate study, provisionally known as the PSACOIN Level S exercise.

Finally, it should be noted that an integral part of this type of intercomparison is the opportunity afforded participants to identify possible errors and misinterpretations associated with their codes. In the Level 0 exercise, four iterations were required before a comparable set of results was obtained (NEA PSAC User Group, 1987). In this exercise, two iterations were

required. After the first iteration, participants were given an opportunity to provide corrections to their results. In the event, several participants, on the basis of a preliminary comparison of their results with those provided by other participants, were able to identify errors in their codes, or in the implementation of their codes, and provided "corrected" results for inclusion in the final analysis presented here.

1.2 Problem Specification

The detailed case specification for the Level E exercise is reproduced in Annex A, together with the questionnaire used to obtain results in a standard form, and tables of exact results (Oldfield et al., 1988). The Level E case specification is designed to represent deep geologic disposal concepts within the limits imposed by the available analytical solution technique of Robinson and Hodgkinson (1987). The repository itself is represented without any consideration of spatial structure or chemical complexities. After a delay representing primary containment failure, the release of radionuclides to the geosphere depends only on leach rate and inventory (modified by radioactive decay). The released radionuclides are transported by groundwater through two geosphere layers with different hydrogeological properties. This process is modelled using a one-dimensional convective-diffusive transport equation in a semi-infinite porous medium. Radionuclides leaving the geosphere enter a stream from which the critical group obtains drinking water. Figure 1.1 illustrates the entire system.

The model has a total of 33 parameters, 12 of which are taken as randomly sampled variables (except in deterministic analyses). Four radionuclides are included: I-129, and the decay chain Np-237 - U-233 - Th-229 (called the Neptunium chain in this report). The overall consequence values (dose rate to a member of the critical group as a function of time) are obtained by convoluting the source outputs with the responses of the two geosphere layers and, finally, multiplying by time-independent factors representing biosphere dilution and radiological exposure efficiencies.

The Level E system model is only partly representative of current assessment models, and its limitations are readily apparent. In particular, formal code verification is limited primarily to the executive functions of PSA codes and to the radionuclide transport submodels of these codes. The transport model specified is currently widely used in PSA codes for radioactive waste disposal. In this sense, the exercise represents a step toward verification of codes that may be used in formal safety assessments.

The results questionnaire (see Annex A) provided the required common PSA code outputs. For deterministic analyses, detailed results were requested for three simulations in which all parameter values were fixed (Section B of the questionnaire). Wherever available, the exact solution was provided in the questionnaire in order to enable participants to confirm that they had correctly coded the system model. For stochastic analyses, requested results included estimates of the mean and standard deviation of dose at several specified times, and of the maximum dose up to various time points (Section C of the questionnaire).

1.3 Participants

Twelve contributions were received from 10 participants (two participants submitted two results questionnaires). Table 1.1 identifies all participants, and summarises the code used, the sampling scheme followed, and the sample size and time steps used. Annex B contains brief descriptions of the various codes used. Table 1.1 also includes a unique letter for each contribution, to identify it in the figures provided in Sections 2 and 3 of this report. Tables of original results from the 12 case studies contributed by participants are not included in this report, but these data are freely available from the NEA Data Bank in both paper and machine-readable format.

Fig. 1.1 Schematic illustration of the Level E system model.

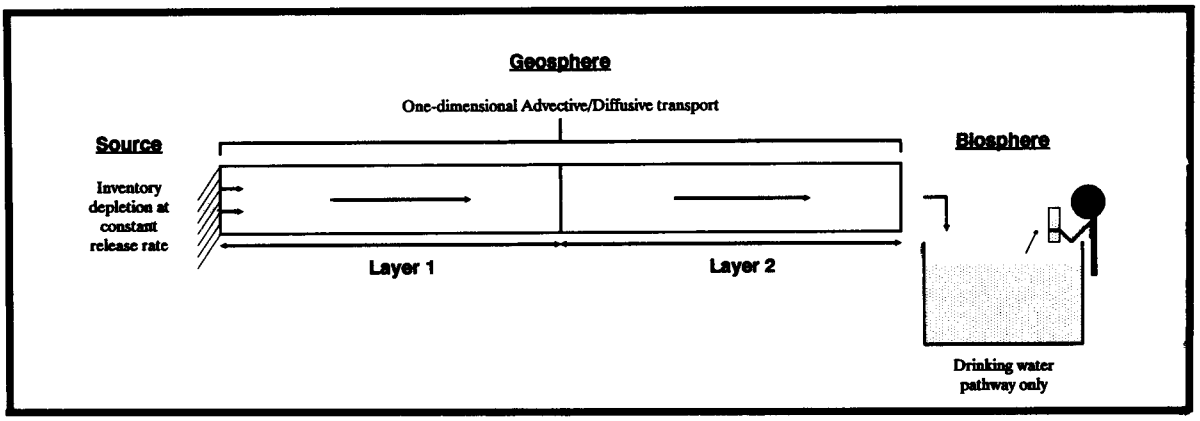


Table 1.1 PSACOIN Level E contributions - summary of Section A of the questionnaire.

Organisation	Country	Letter Used	Method	Program	I^{129} Nr. of Runs	Np^{237}-Chain Nr. of Runs	Time Steps
INTERA	United Kingdom	A	Exact	ESCORT			
CEN/SCK	Belgium	B	LH	LISASCK-4.0E	200	200	140
UKDOE	United Kingdom	C	IS	SYVAC-D/1.0		1000	201
UKDOE	United Kingdom	D	MC	SYVAC-D/1.0	1000	10000	201
AERE-H	United Kingdom	E	MC	MASCOT-PRAM2D	1000	1000	
AERE-H	United Kingdom	F	MC	MASCOT-PRAM2D	4000	4000	
JAERI	Japan	G	LH	JAERI-LHS/1.1	3000	3000	
AECL-CR	Canada	H	MC	COSMOS-E	500		500
SKI	Sweden	I	MC	SYVAC/SU-2	800	800	
SKB	Sweden	J	MC	PROPER-0.0	1000	1000	adaptive
NRPB	United Kingdom	K	LH	ESP-88	500	500	>200
CEC/JRC	European Comm./Spain	L	MC	LISA4-JRC	942	1215	1000
		M		Withdrawn			
AECL-W	Canada	N	MC	SYVAC3-LE1	1000	1000	10-400

Sampling Methods: MC Monte Carlo, LH Latin Hypercube, IS Importance Sampling

2. DETERMINISTIC RESULTS

Section B of the case-study questionnaire elicited three different sets of deterministic results. The deterministic results allowed participants to ensure that particular submodels used were both suitable and correctly implemented. It was considered that such preliminary analyses done by the participants themselves would help ensure that most of the discrepancies observed in the stochastic results would be due to statistical effects.

2.1 Comparison with Exact Solution

For each of the three deterministic cases, the participants were asked to supply for each of the four radionuclides involved

(1) flux from the source at 10^3 a (for I-129) and 10^5 a (for the Neptunium chain),

(2) maximum flux at the end of layer 1 and time of occurrence, and

(3) maximum dose and time of occurrence.

The principal code output consists of dose but, in order to help locate the sources of possible errors, intermediate results were also requested. Figures 2.1 to 2.8 show representative results, as well as the exact solution (continuous or broken lines) for the three cases. Because there are many overlapping values on the scale of these figures, Figs. 2.1(b), 2.2(b), 2.3(b), and 2.5(b) have an expanded scale focussed on the area of peak doses.

For deterministic case 1, peak doses from I-129 and I-129 fluxes from geosphere layer 1 and the source are plotted versus time in Figs. 2.1, 2.2 and 2.3, respectively. These figures show that with the exception of results from the COSMOS-S/D code, differences between the contributed results, and between these results and the exact solution, are relatively small. The COSMOS-S/D code provided systematically high estimates of both peak dose and layer 1 flux, which may be due to the relatively large time steps (100 and 1000 a, see Annex B) used to conduct the simulation. For the results from the remaining codes, the most notable feature is the excellent agreement in estimates of both peak dose and layer 1 flux, compared to the somewhat poorer - but still adequate - agreement in estimates of time of occurrence for these peaks.

Peak doses from I-129 for deterministic cases 2 and 3 are plotted versus time in Figs. 2.4 and 2.5, respectively, and from the Neptunium chain for deterministic cases 1, 2 and 3 in Figs. 2.6, 2.7 and 2.8, respectively. The agreement, although still excellent for the majority of participants, is somewhat poorer for some participants. In particular, the SYVAC/SU and LISA.SCK codes produced slightly divergent results for both I-129 cases, in addition to the systematically high peak dose estimates provided by the COSMOS-S/D code (Figs. 2.4 and 2.5). The COSMOS-S/D code did not provide

results for the Neptunium chain, and the only notably divergent peak dose estimates were provided by the SYVAC-D and LISA.SCK codes, both of which moderately underestimated peak doses from parts of the Neptunium chain in deterministic case 3 (Fig. 2.8). For all of these figures (2.4 to 2.8) again, however, it can be observed that nearly all participants provided excellent estimates of peak doses, in comparison to the somewhat greater divergence in the estimates of time of occurrence for these peak doses.

The discrepancies shown in Figs. 2.1 to 2.8, both between codes and with the exact solution, might be attributable to any number of the following possible causes.

(1) Level of modification of the code. Some participants chose to run the exercise with minimum changes to their existing system models, so that they would also be verifying code intended for direct use in their formal safety assessments. Other participants were required to develop a suitable system model to meet the problem specification.

(2) Time stepping. Most codes obtain a solution by stepping progressively forward in time, with methods ranging from fixed time steps to adaptive time steps to variable but user-defined time steps. This variation can affect the accuracy of results for two reasons: first, because of the need to interpolate values for a specific requested time and, second, because time-step sizes and their possible variation from one submodel to the next affect the accuracy of convolution of submodel responses.

(3) Spatial discretisation. In some codes, numerical solution of the one-dimensional transport equation requires subdivision of layers into cells. The cell size affects accuracy in a manner which is analogous to, and strongly interactive with, the time stepping.

(4) Secular equilibrium. Some participants assumed that Th-229 was in secular equilibrium with U-233, whereas others solved the required set of three coupled partial differential equations. This difference should not greatly affect some results; for example, for the three deterministic cases, secular equilibrium is a good assumption.

(5) Coding Errors. While it is expected that all participants have been assiduous in checking for possible errors within their codes, some errors could still remain. Some errors might be detected only under unusual conditions, and affect the stochastic but not the deterministic simulations.

It should be noted that only peak fluxes and doses were compared in this exercise. It can be speculated that comparison of additional information, such as fluxes or doses at several times, would have shown a similar level of agreement (and discrepancy) as that evidenced in Figs. 2.1 to 2.8. It is recommended, however, that questionnaires for future PSACOIN exercises elicit plots of consequence versus time in a well-defined format. Such information could prove valuable during preliminary comparison of the quality of results, particularly for comparisons involving complex system models.

2.2 Principal Component Analysis

Figure 2.9 shows a principal component analysis (PCA) of the variation among participants' deterministic results. This analysis allows an easy visualisation of any systematic differences between sets of results; the analysis does not, however, imply that outlying data are incorrect. Appendix B of the Level 0 report (NEA PSAC User Group, 1987) contains details of how the PCA technique is applied to code intercomparisons of this kind (see also Chatfield and Collins, 1983). Unlike the comparison methods discussed elsewhere in this report, which analyse discrepancies observed in small subsets of the result variables, PCA examines the global agreement among the participants' results.

In Fig 2.9, several codes appear to be outliers from all others, including the exact solution (labelled with the letter A), with, on the whole, just those codes that provided relatively divergent estimates for some of the peak doses being the furthest outlying, i.e., the SYVAC/SU, SYVAC-D, and LISA.SCK codes. In addition to these three codes, the LISA-JRC code appears to be a relative outlier. Note, however, that results for the COSMOS-S/D code do not appear in this particular analysis.

Part of the dispersion observed in Fig. 2.9 is due to the amplification of discrepancies in this PCA arising from differences in the estimation of the time of occurrence of peak dose. Figures 2.1 to 2.8 show that several participants' codes have identified the time of occurrence of maxima with relatively low accuracy compared to their estimation of the maximum doses themselves, but that their results are nonetheless consistent with the exact solution because of the relative flatness of the dose-time curve at the time of peak dose.

To conclude, because it is difficult to place any absolute limits upon what degree of discrepancy is acceptable, no code has been disqualified from consideration in the stochastic analyses. In other words, none of the discrepancies observed in Fig. 2.9 are considered to be particularly significant at this point in the analysis.

Fig. 2.1a Peak dose from I-129 versus time for deterministic case 1, showing a full range for the exact solution. Note that not all results are included here, although they are in Fig. 2.1b below.

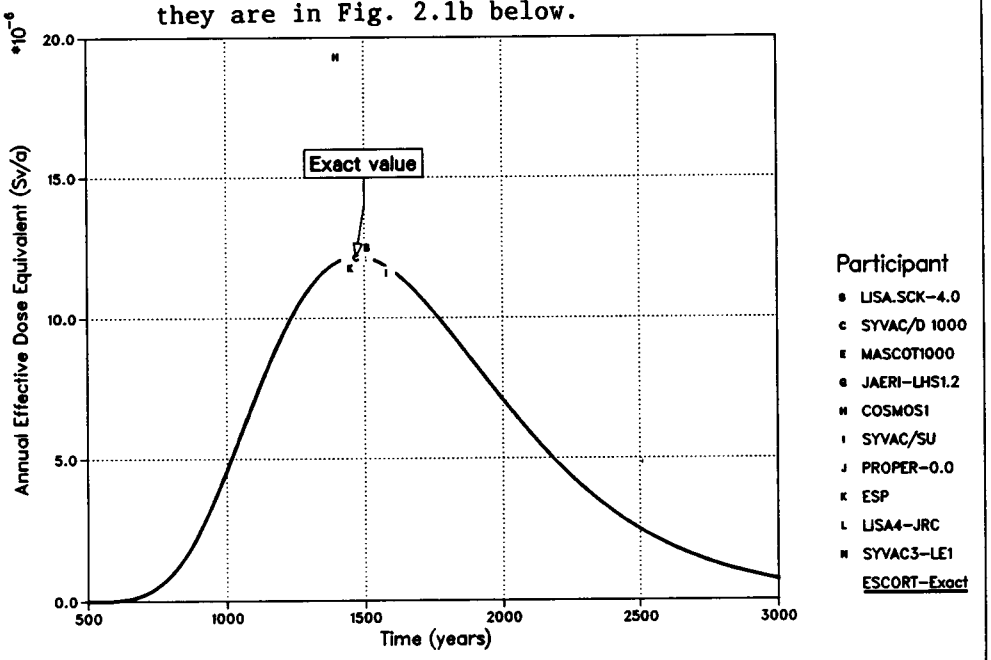


Fig. 2.1b As Fig. 2.1a, but showing an expanded area focussed on the peak doses. Note that results G and L overlap with E.

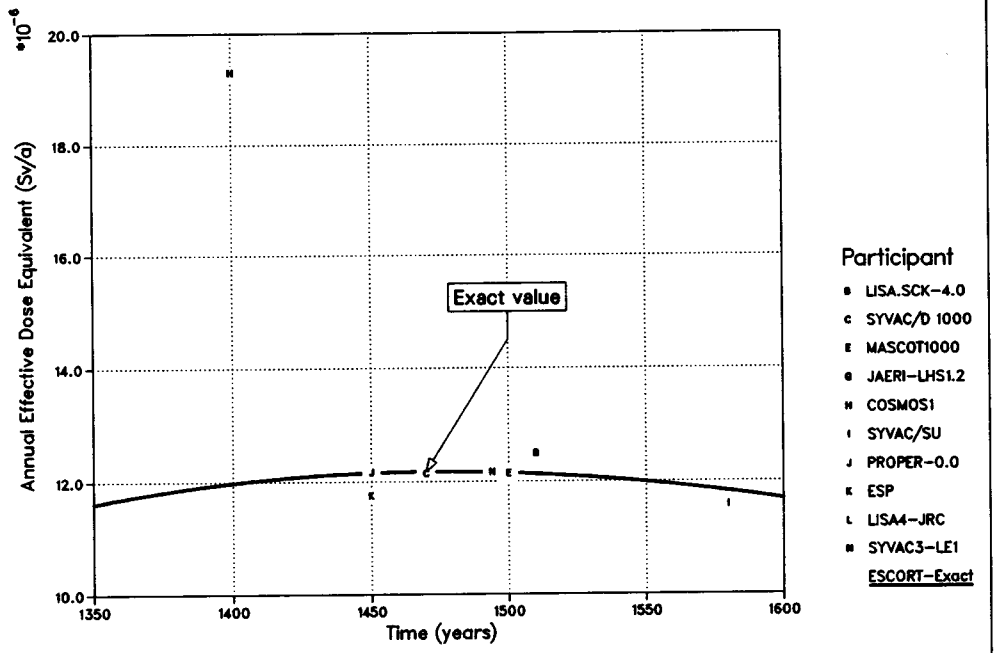


Fig. 2.2a Peak I-129 flux from geosphere layer 1 versus time for deterministic case 1, showing a full range for the exact solution. Note that not all results are included here, although they are in Fig. 2.2b below.

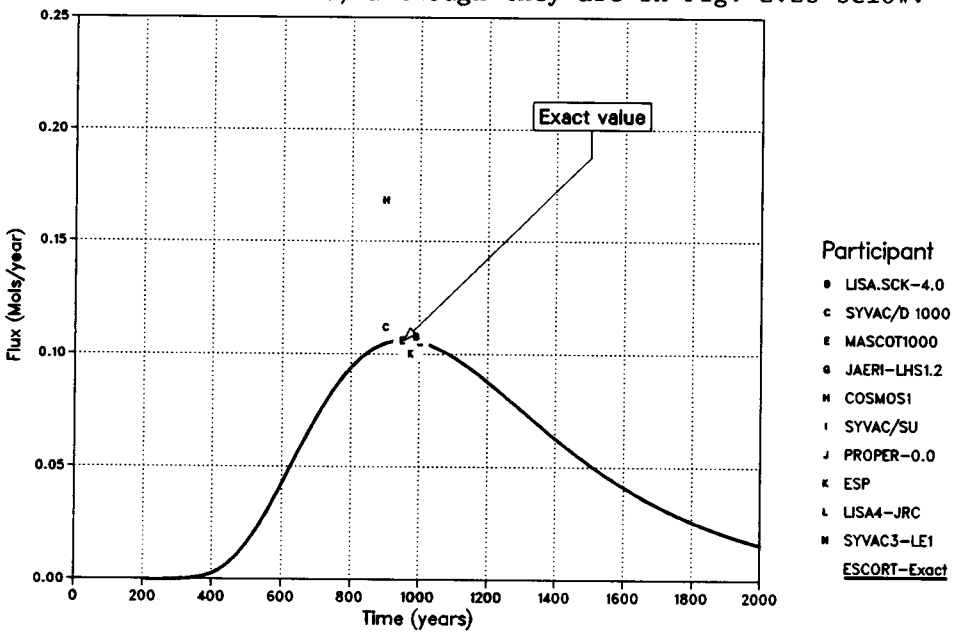


Fig. 2.2b As Fig. 2.2a, but showing an expanded area focussed on the peak fluxes. Note that result I overlaps with G.

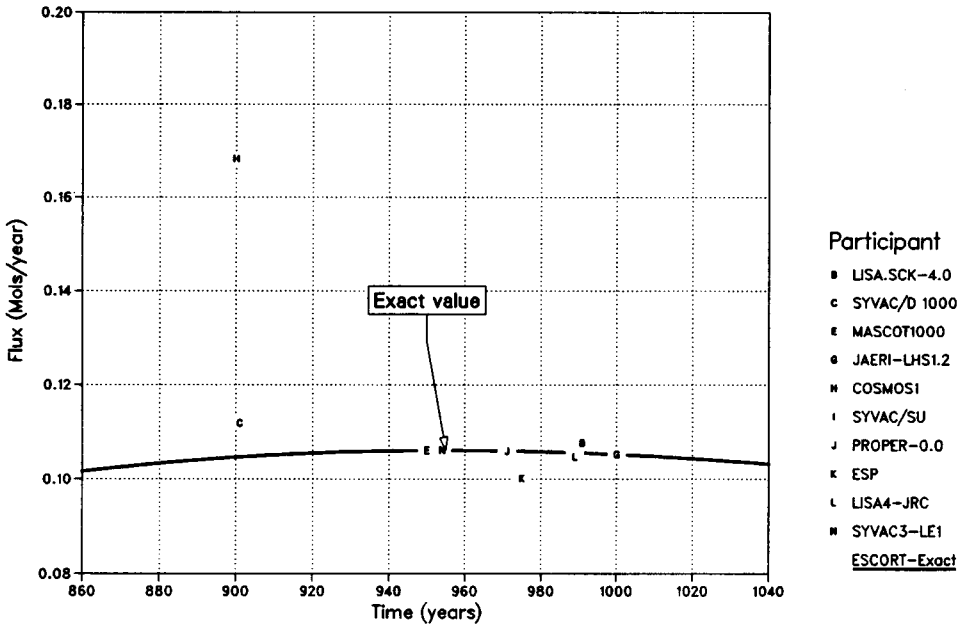


Fig. 2.3 I-129 flux from source versus time for deterministic case 1. Note that results D, E, F, G, H, I and L overlap with B.

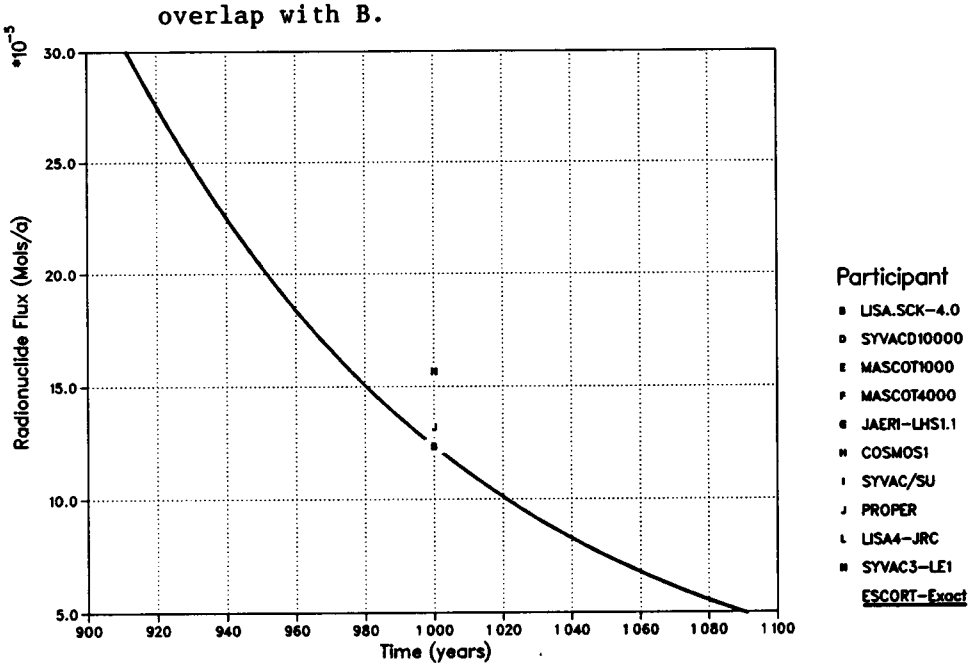


Fig. 2.4a Peak dose from I-129 versus time for deterministic case 2, showing a full range for the exact solution. Note that not all results are included here, although they are in Fig. 2.4b below.

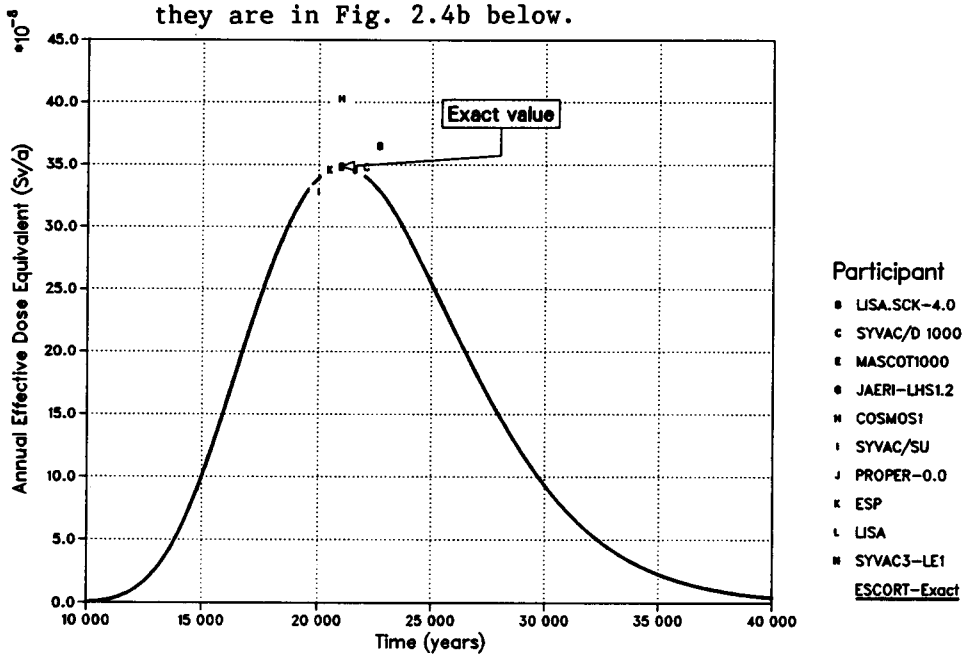


Fig. 2.4b As Fig. 2.4a, but showing an expanded area focussed on the peak doses. Note that result N overlaps with E.

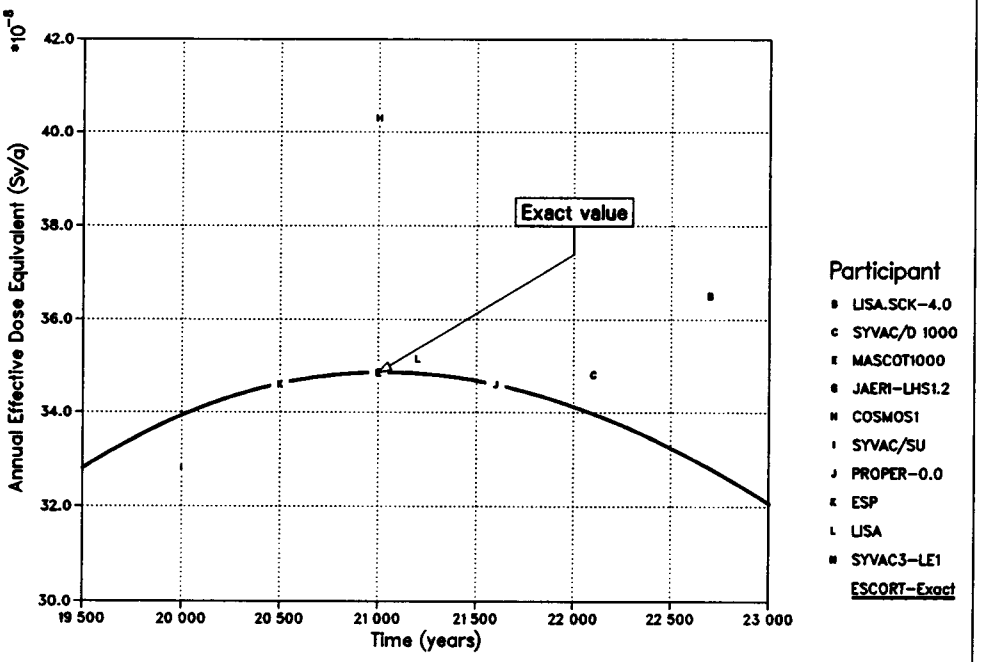


Fig. 2.5a Peak dose from I-129 versus time for deterministic case 3, showing a full range for the exact solution. Note that not all results are included here, although they are in Fig. 2.5b below.

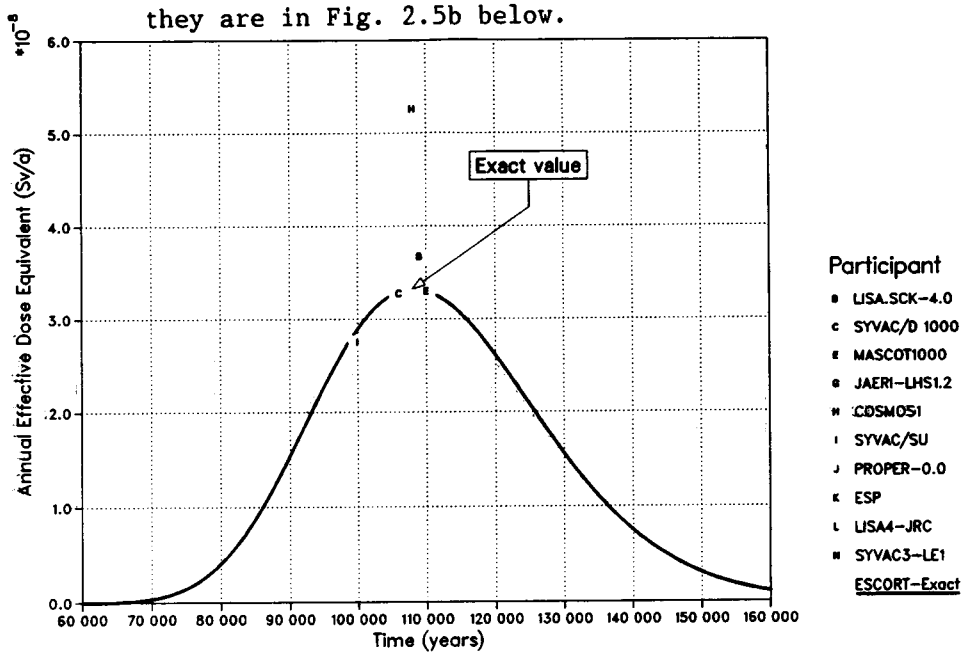


Fig. 2.5b As Fig. 2.5a, but showing an expanded area focussed on the peak doses. Note that result G overlaps with E and result K overlaps with C.

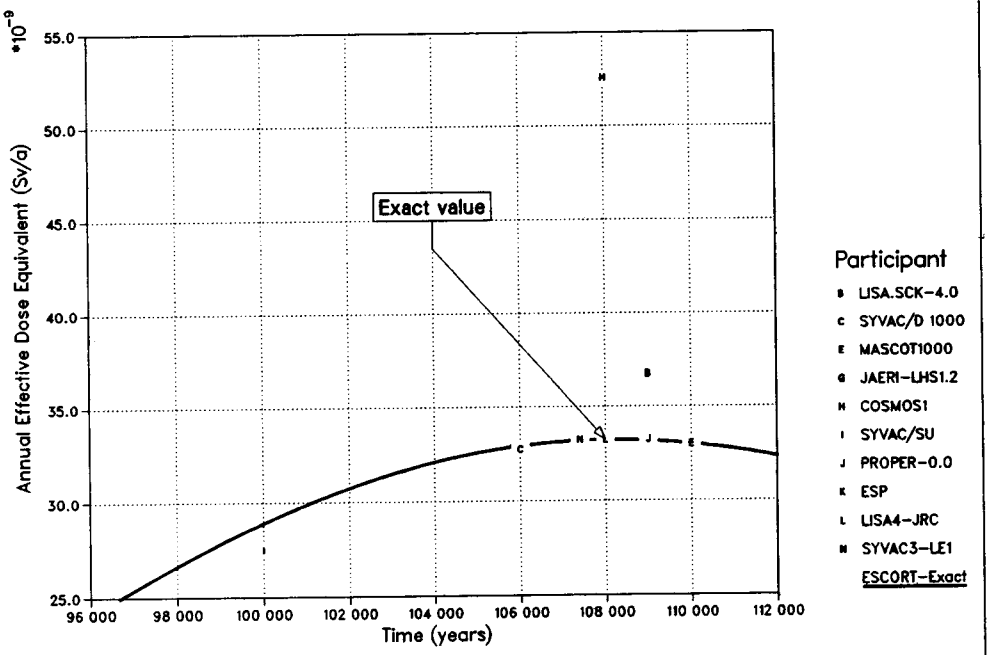


Fig. 2.6 Peak dose from the Neptunium chain versus log-time for deterministic case 1.

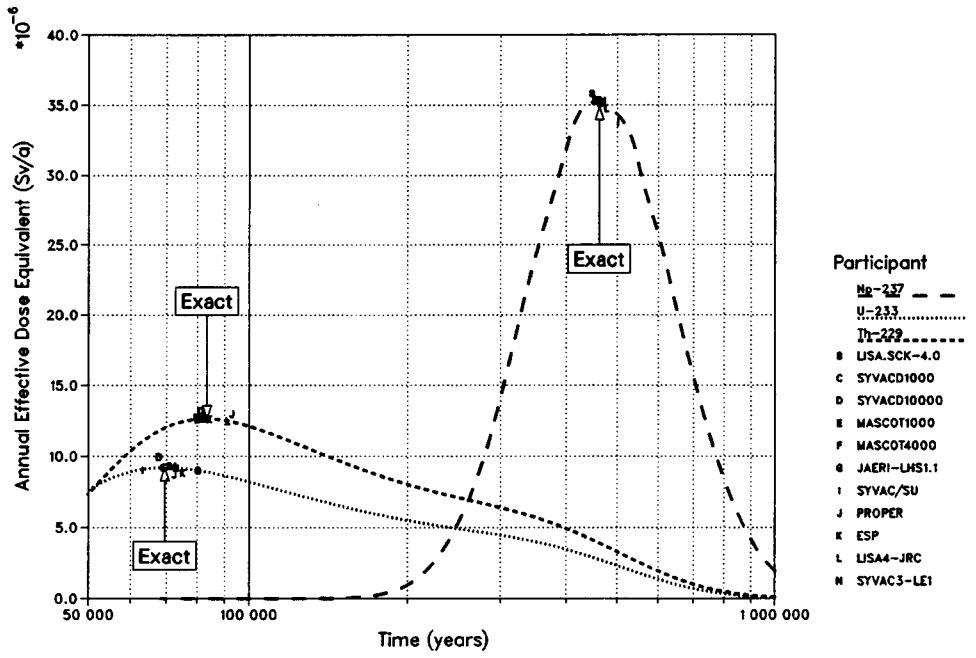


Fig. 2.7 Peak dose from the Neptunium chain versus log-time for deterministic case 2.

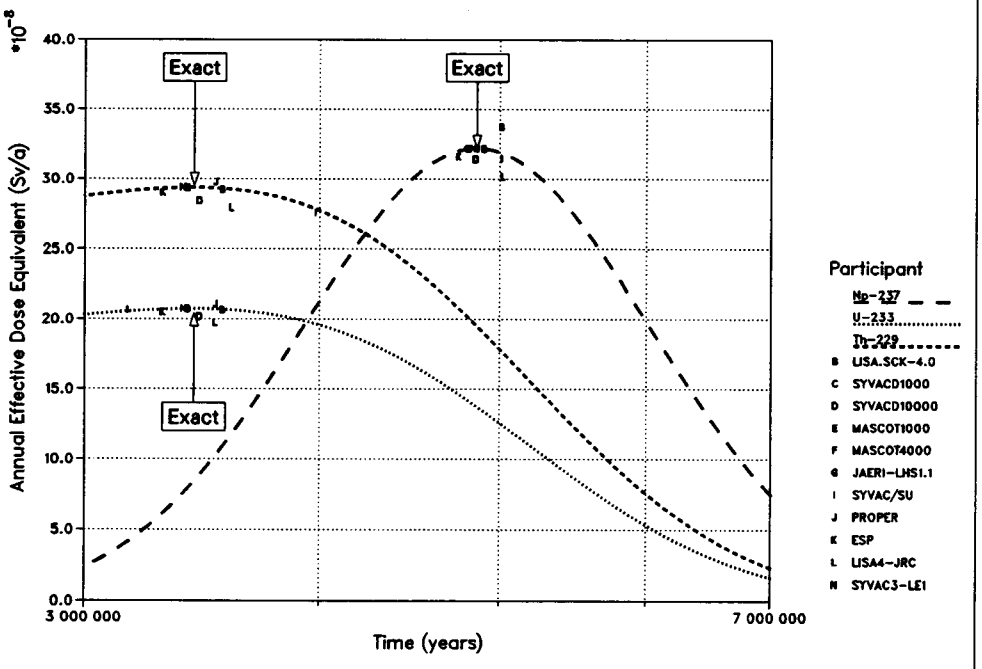


Fig. 2.8 Peak dose from the Neptunium chain versus log-time for deterministic case 3.

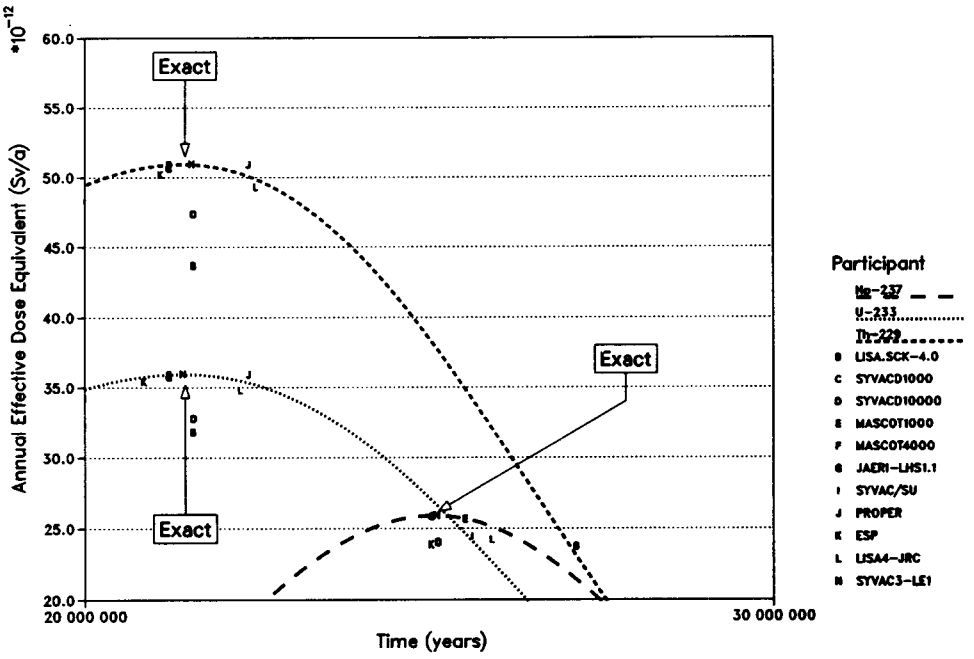
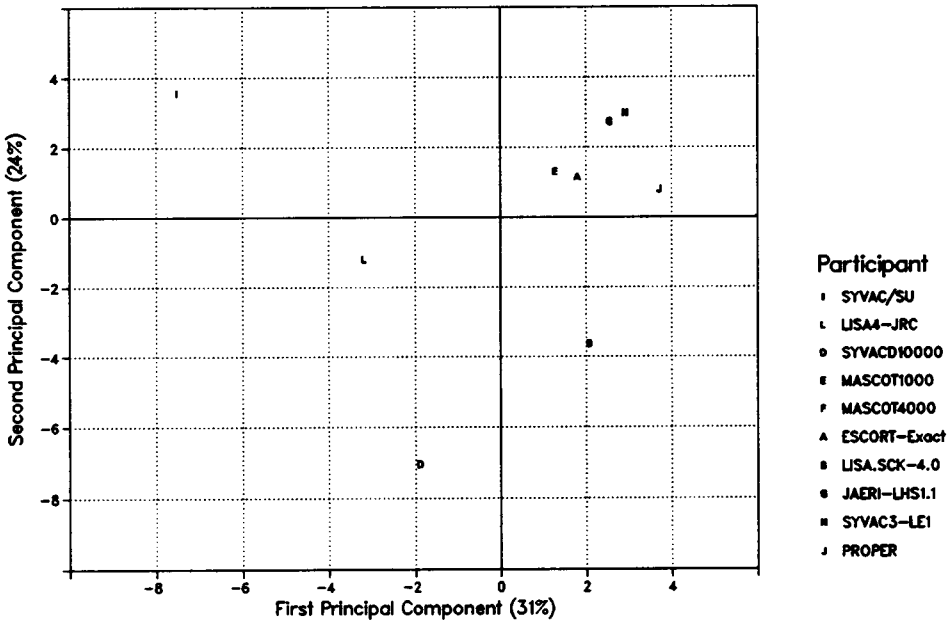


Fig. 2.9 PCA for all deterministic variables showing the first (31%) and second (24%) principal components. Note that result F overlaps with E, and that participants C, H and K are not included because they did not submit complete sets of deterministic results (see Section 2.2 for explanation).



3. STOCHASTIC RESULTS

Section C of the case-study questionnaire elicited a number of representative statistical measures of the performance of the model system. These mainly concentrated on descriptions of the distribution of dose resulting from the assumed distributions of the model parameters. Exploration of the dependence of dose on individual parameters was not covered at all. On the other hand, a number of the requested results relate to the important matter of the accuracy of the mean dose estimates, and how these converge as sample size increases.

For the expected mean value of dose at a given time, the exact solution provided reference values with which each participant's results could be compared. For other quantities, only comparisons amongst the PSA code results was possible, because the analytic integrals used in the exact solution are readily tractable only for linear operators.

The estimation of means and standard deviations depends to some extent on the parameter sampling strategy in use. Three strategies were represented in the contributed results: simple Monte Carlo sampling (MC), Latin Hypercube Sampling (LHS), and Importance Sampling (IS). In addition, two types of confidence intervals were examined: "Chebyshev" and "normal", with the latter being examined for validity by the Shapiro-Wilk test.

3.1 Theory

Before presenting and discussing the stochastic results, it will be useful to set out the equations that participants used to provide the requested statistical results, and to clarify some often confusing points regarding variances of dose and of mean estimators. In what follows, the model parameters that are sampled are represented by the vector $\underline{p}$, and $y(\underline{p})$ is considered the dependent quantity (e.g., dose at time or maximum dose up to time) whose statistics are being calculated. Individual samples of parameter values are labelled by the index n, which ranges from 1 to N.

3.1.1 Means

For both MC and LHS, the estimator for a mean is

$$E_e(y) = \bar{y} = \frac{1}{N} \sum_n y(\underline{p}_n), \qquad (3.1)$$

where $E_e(y)$ is an estimate of E(y), the true expectation value of the probability density function of $y(\underline{p})$ implied by the specified distribution functions for the parameters, $\underline{p}$.

With IS, the formula is modified to

$$E_e(y) = \overline{wy} = \frac{1}{N} \sum_n w_n y(\underline{p}_n), \qquad (3.2)$$

where the weights, w_n, are obtained from the ratio of the true joint probability density for the parameters, $f(\underline{p})$, to the probability density used in selecting sample parameter sets, $g(\underline{p})$:

$$w_n = f(\underline{p}_n) \; / \; g(\underline{p}_n). \qquad (3.3)$$

Under their respective conditions of sampling, Eqns. (3.1) and (3.2) both represent "unbiased" estimators for E(y) (e.g., Hogg and Craig, 1978). Unbiased means that the mathematical expectation value of the expression for $E_e(y)$ is equal to E(y) or, in other words, if infinitely many different sets of N samples were taken, the values obtained for $E_e(y)$ would vary, but their mean would equal E(y).

3.1.2 Standard Deviations

For all sampling schemes, the estimator for standard deviation is obtained as the square root of an estimator for variance:

$$\sigma_e(y) = [V_e(y)]^{\frac{1}{2}}. \qquad (3.4)$$

For both MC and LHS, an unbiased estimator for the variance of $y(\underline{p})$ is

$$V_e(y) = \frac{N}{(N-1)} [(\overline{y^2}) - (\overline{y})^2)]$$

$$= \frac{N}{(N-1)} \left\{ \frac{1}{N} \sum_n [y(\underline{p}_n)]^2 - [E_e(y)]^2 \right\}. \qquad (3.5)$$

The factor (N/N-1) is strictly necessary to remove bias, but is not particularly important with sample sizes of hundreds or thousands, as used in this exercise.

For IS, an unbiased estimator for the variance of $y(\underline{p})$ is

$$V_e(y) = \frac{N}{N-1} [(\overline{w})(\overline{wy^2}) - (\overline{wy})^2] \qquad (3.6)$$

$$= \frac{N}{N-1} \left\{ \frac{1}{N^2} \sum_n w_n \sum_n w_n [y(\underline{p}_n)]^2 - [E_e(y)]^2 \right\}.$$

$V_e(y)$, the estimated variance of y, should not be confused with the variance of the estimator, $E_e(y)$, for the mean of y. All sampling schemes should provide similar values of $V_e(y)$ and, hence, $\sigma_e(y)$, because these are estimates of V(y) and $\sigma(y)$, properties of the distribution of the dependent variable, y. $V_e(y)$ will be large or small only according to the width of the distribution of y. On the other hand, the estimator, $E_e(y)$, may have a different variance for different sampling schemes and for different values of N, the total number of samples. The smaller the variance of this estimator, the higher the probability that the estimate will be close to the actual value of the quantity being estimated.

3.1.3 Confidence Intervals

Confidence intervals are a means of expressing the likely difference between an estimate, $E_e(y)$, of the mean of a quantity, y, and the actual mean, E(y). Bounds on the likely error can be determined at a certain level of confidence on the basis of the variance of the estimator, although in principle further more-detailed knowledge of the underlying distribution could be used if available. Confidence intervals were used in the Level E exercise to investigate possible differences in sampling-scheme efficiency.

With the MC sampling scheme, the estimator $E_e(y)$ given in Eqn. (3.1) has variance

$$V\,[E_e(y)] = V(y)/N, \tag{3.7}$$

where V(y) is the true variance of y. This follows because Eqn. (3.1) is a summation over independent samples, $y(\underline{p}_n)$, from the same distribution. Since V(y) is unknown, $V_e(y)$ [Eqn. (3.5)] was used for obtaining confidence intervals.

With the IS scheme, the estimator $E_e(y)$ in Eqn. (3.2) has variance

$$V\,[E_e(y)] = V(wy)/N, \tag{3.8}$$

because each $w_n y(\underline{p}_n)$ is an independent sample from the same distribution. Since wy is as much a random variable as y itself, its variance can be estimated, by analogy with Eqn. (3.5), as

$$V_e(wy) = \frac{N}{N-1}\,[(\overline{w^2y^2}) - (\overline{wy})^2]. \tag{3.9}$$

With the LHS scheme, there is not a convenient formula for the variance of the estimator, $E_e(y)$, although McKay et al. (1979) gave an expression involving the means of y in each of the hypercube cells into which the parameter space has been divided. They used this expression to prove that the variance of $E_e(y)$ is smaller than would be obtained using MC sampling with the same number of samples. The proof only holds, however, when $y(\underline{p})$ is a monotonic function of every component of $\underline{p}$ (i.e., of each independently sampled model parameter). In addition, there is no general theory for the actual amount by which the variance would be reduced. Thus, although for many applications LHS may well provide more accurate estimates than MC sampling,

these estimates are unsupported by quantitative confidence intervals, so the degree of its advantage over MC sampling is unknown.

As explained in the case specification (see Annex A, Section 3.1), Chebyshev's Inequality can be used to give

$$E_e(y) \pm 4.47 \{ V[E_e(y)] \}^{\frac{1}{2}} \qquad (3.10)$$

for a 95% confidence interval on $E_e(y)$, the estimated mean of y (Saltelli and Marivoet, 1988). The smaller interval,

$$E_e(y) \pm 1.96 \{ V[E_e(y)] \}^{\frac{1}{2}}, \qquad (3.11)$$

is appropriate when the estimator, $E_e(y)$, is normally distributed. This condition should in principle be approached as the number of samples increases. To establish whether $E_e(y)$ was, at least approximately, normally distributed, the Level E questionnaire invited participants to apply the Shapiro-Wilk test (see Annex A, Section 3.1.2).

Finally, it should be noted that a member of the PSAC User Group has recently indicated that confidence intervals based on an analysis of Guttman and intermediate in size between those given by Eqn.'s (3.10) and (3.11) can be used with MC sampling, without any assumptions of normality (Woo, 1989). This information was, however, provided too late to be included in the Level E exercise.

3.2 Means and Standard Deviations

Estimates were requested for the mean and standard deviation of the following quantities:

(1) dose rate (Sv/a) from I-129 at times 1×10^4, 2×10^4, 5×10^4, 1×10^5, 2×10^5, and 5×10^5 a (question C1),

(2) maximum dose rate from I-129 up to the same set of time values (question C2),

(3) total dose rate from the Np-237 - U-233 - Th-229 chain at times 5×10^5, 1×10^6, 2×10^6, 5×10^6, and 1×10^7 a (question C3), and

(4) maximum dose rate from the chain up to the same set of time values (question C4).

Figures 3.1 to 3.6 show most of these results, together with results from the exact solution where available. Figures 3.1 and 3.2 show mean doses versus time from I-129 and the Neptunium chain, respectively, whereas Figs. 3.3 and 3.4 show maximum doses up to specific times from I-129 and the Neptunium chain, respectively. Standard deviations, corresponding to the dose data shown in Figs. 3.1 and 3.2, are illustrated in Figs. 3.5 and 3.6, respectively.

3.2.1 Mean Dose

In Figs. 3.1 and 3.2, the estimated means can be compared with each other and with the exact result. In Fig. 3.1 for I-129, the estimates tend to cluster around the exact result, with the exception of one relatively outlying set. The outlying data set was obtained with the COSMOS-S/D code, using relatively large time steps to conduct the simulation, which, as already noted in Section 2, may have led to a systematic error in the results for this code. For the remaining results, the only noticeable trend in Fig. 3.1 is that the spread is larger at earlier times than at later ones. The likely explanation is that at early times, the mean dose arises from a small fraction of cases which produce large doses; the statistics are therefore "poorer" than at late times, when for almost all sample cases the peak dose has been passed, and the average is over a large number of decaying "tails". However, neither spurious statistical effects nor problems with the codes themselves can be ruled out as possible explanations for this trend.

Similar remarks apply to Fig. 3.2 for the Neptunium chain, except that the tendency for the spread between estimates to decrease at later times is not as strong as was the case for the I-129 results (but note the different scales for both the time and dose axes of Figs. 3.1 and 3.2). A further interesting feature is that at the earliest time, 5×10^5a, the estimates of mean dose are all smaller than the exact value. It would be fortuitous for dose underestimation at early time to be peculiar to the Neptunium-chain results and, it is therefore reasonable to speculate that dose underestimation would have also been seen for the I-129 results had a sufficiently early time point been included in the exercise. The likely explanation is again that the true mean at early times is contributed to by only a small fraction of cases: relatively rare parameter combinations give rise to very large doses, whereas the remainder give essentially zero dose. These contributing parameter combinations occupy such a small fraction of parameter space that most calculations over a few hundred or even a few thousand sample cases will inadequately represent them, and hence underestimate the mean dose. Yet here again, neither spurious statistical effects nor problems with the codes themselves can be ruled out as possible explanations.

At first sight, explanations in the preceding paragraph may seem to contradict statements in Section 3.1 of the report that Eqns. (3.1) and (3.2) are unbiased estimators, regardless of sample size. There is in fact no contradiction, although the distinction is subtle. The estimator $E_e(y)$ is unbiased only in the sense of having expectation value equal to the true value of the mean being estimated, not in the sense that it will overestimate half the time and underestimate half the time. Indeed, with the underlying dose distribution being skewed toward small values, $E_e(y)$ undoubtedly underestimates the true mean value more frequently than it overestimates it. When overestimates do occur, however, they are presumably by larger margins than those of the more common underestimates. For the Neptunium-chain dose at 5×10^5 a, all of the 11 contributed estimates presumably fall into the more common class of underestimates (Fig. 3.2).

3.2.2 Mean Values of Maximum Dose up to Given Times

Figures 3.3 (for I-129) and 3.4 (for the Neptunium chain) illustrate the expected trend for the mean value of maximum dose up to a given time to increase monotonically with time, approaching asymptotically the mean value of maximum dose over all time. Note that the relative size of the spread amongst results is slightly larger for the Neptunium-chain than for the I-129 contributions. Note also that the COSMOS-S/D code, which provided the largest doses in Fig. 3.1, did not supply results for maximum dose up to time, and is missing from Fig. 3.3. For the remaining codes, there is no significant correlation between the ordering of results for mean dose at time (Fig. 3.1) and mean of maximum dose up to time (Fig. 3.3); the scatter in these figures is, therefore, consistent with a purely statistical origin. The only possibly deviant set of results is from the PROPER code, which provided relatively high estimates of mean of maximum dose up to time for the Neptunium chain (but not for I-129).

3.2.3 Standard Deviation of Dose

The spread of results for standard deviation of mean dose at given times for both I-129 (Fig. 3.5) and the Neptunium chain (Fig. 3.6) shows a qualitative similarity to those for the corresponding mean-dose results (Figs. 3.1 and 3.2). In particular, standard deviations of doses obtained with the COSMOS-S/D code are relatively high at just those earlier times when the same code produced relatively high estimates of mean dose. Other corresponding data pairs can, however, be easily identified. Plots of standard deviations for the dose data shown in Figs. 3.3 and 3.4 are not included here because they do not provide additional insight for the intercomparison to that provided by Figs. 3.5 and 3.6.

3.2.4 Discussion

For the means of maximum dose up to time (Figs. 3.3 and 3.4), and for estimates of standard deviation (Figs. 3.5 and 3.6), there is no exact solution to compare with, so it cannot be discerned on this basis whether the estimated values are either too large or too small. The above discussion on overestimation and underestimation of means, however, suggests that underestimation of any quantity is likely to be more frequent when it is a mean of a sample drawn from a distribution that is highly skewed toward small values. Because the standard deviations of dose involve the mean square of dose, whose distribution would be even more skewed that that of dose, it is possible that too small a sample size would tend to produce underestimates of the standard deviations even more than of the means.

In the absence of any exact solution for standard deviation, it was difficult to examine this possibility with any reliability. In one attempt, all of the submitted σ_e values (for various times, and both I-129 and Neptunium-chain contributions) were collectively examined, dividing each by the global average (from all participants) to provide a normalised measure of overestimation or underestimation. Plotting the results against the sample size used revealed no systematic trend. In particular, there was no indication of a minimum sample size below which σ_e values were obviously unreliable.

The overall conclusion with regard to the intercomparison of means and standard deviations is, then, that there are no signs of systematic deviations from either the exact solution (where available) or the consensus of other codes, except in one case (the COSMOS-S/D code), where a possible explanation has been given. The remaining differences appear to be consistent with the statistical variation to be expected from the use of independent sets of sampled model parameters.

3.3 Confidence Intervals

Questions C1 and C3 of the case-study questionnaire asked for confidence intervals to be given for the estimates of mean dose at selected times for I-129 and the Neptunium chain, respectively, whereas questions C7 and C8 were restricted to a single time point (2×10^4 a for I-129 and 2×10^6 a for the Neptunium chain), but asked for the means and confidence intervals to be given as a function of the number of samples. In addition, Section 3.1 of the case-study specification gave two methods of computing confidence intervals - based on Chebyshev's Inequality and the Shapiro-Wilk statistic - and invited participants to suggest further methods. No further methods were, however, contributed.

Results selected for presentation in this Section of the report are drawn from questions C7 and C8, and from just those time points in C1 and C3 that correspond to those used in C7 and C8. Because all of the confidence intervals should vary proportionally to the inverse square root of the sample size, N (see Section 3.1.3), all results have been plotted against $N^{-\frac{1}{2}}$. Figures 3.7 and 3.8 show the means and Chebyshev 95% confidence intervals for the dose from I-129 at 2×10^4 a and from the Neptunium chain at 2×10^6 a, respectively. Figure 3.9 shows the values of the Shapiro-Wilk statistic, W, for I-129 at 2×10^4 a, and Fig. 3.10 shows the means and normal 95% confidence intervals for the same case. The normal confidence intervals in Fig. 3.10 have been plotted regardless of their validity as indicated by the Shapiro-Wilk statistic.

3.3.1 Chebyshev Confidence Intervals

The Chebyshev confidence intervals are not based upon any assumptions with regard to the shape of the underlying dose distribution. It was expected, therefore, that these intervals would provide a conservative basis for bounding those uncertainties in estimated mean dose values that arise from the limited sample size in a PSA calculation.

Examination of Figs. 3.7 and 3.8 leads to a number of relevant observations. It can be seen that the expected trend for confidence intervals to grow with $N^{-\frac{1}{2}}$ is broadly confirmed. On the other hand, there is considerable scatter in the intervals calculated for comparable values of N. In particular, some of the intervals for small sample sizes (large $N^{-\frac{1}{2}}$) are disconcertingly small. This might imply that some variances have been underestimated. The danger of small sample sizes is that the estimated variance may be highly inaccurate, resulting in unrealistically small bounds being placed about the mean estimate. It can be seen in Figs. 3.7 and 3.8, however, that in all cases the Chebyshev 95% confidence intervals enclose the exact mean dose value. (Figure 3.10 shows, on the other hand, that in a number of cases, the normal 95% confidence intervals do not embrace the exact mean.)

Finally, it can be seen in Figs. 3.7 and 3.8 that the scatter of mean estimates, for all but the smallest sample size, is somewhat narrower than the consensus envelope of confidence intervals. To summarise, the observations presented here indicate that Chebyshev's Inequality does indeed lead to intervals that are conservatively large. To make this conclusion more reliably, however, would require a larger sample of independent sets of results than those provided in this exercise.

3.3.2 Shapiro-Wilk Confidence Intervals

Narrower confidence intervals than those provided by Chebyshev's Inequality can be said to apply when the sample size is sufficiently large that $E_{\bullet}(y)$ becomes a normally distributed statistic. The difficulty lies in knowing when the sample size is sufficiently large. A test of normality has been advocated by some members of the PSAC User Group, based on the Shapiro-Wilk statistic; this is explained in the case specification (Annex A). Participants were invited to apply the Shapiro-Wilk test and to calculate the smaller, "normal" 95% confidence intervals.

The Shapiro-Wilk test statistic, W, is based on analysis of the means of batches of dose values obtained by subdividing the full sample taken. The expected values of W depend slightly on the number of batches, but this can be ignored as almost all participants used 10 batches. To avoid confusion in Fig. 3.9, points from each participant are not joined by a line, but careful examination of any set shows that the W value varies erratically with N. As indicated in Table 3 of the case specification (Annex A, Section 3.1.2), a W value as low as 0.90 should be obtained with only 20% frequency from 10 samples of a true normal distribution. The data shown in Fig. 3.9 imply, therefore, that in many cases - even with some of the largest sample sizes - the batch means are highly unlikely to be normally distributed. This does not necessarily prove that the mean over the full sample, 10 times larger than each batch, is not a normal statistic. It is, however, sufficient to cast doubt on the use of the normal confidence intervals for this exercise. The failure of some normal confidence intervals in Fig. 3.10 to enclose the exact mean confirms this doubt, although no attempt has been made to find the correlation between such deviation of the intervals and the occurrence of a relatively small W value.

That some of the normal confidence intervals in Fig. 3.10 fail to enclose the exact mean does not indicate that these intervals should never be used. Rather, their use depends upon the estimator for mean being a normally distributed statistic. In addition, the test statistic, W, can be considered useful insofar as small values may provide a warning of the possible lack of conservatism of the normal confidence intervals for a particular case.

The question remains, however, whether the Shapiro-Wilk test is useful in indicating when sufficient samples have been obtained for the normal confidence intervals to be safely applied. In this exercise, many participants found W to oscillate from well above 0.9 to well below it as N was increased. The problem is that a single high value could be mistakenly considered as indicating convergence. For example, if a W of 0.7 is found with 1000 samples, and a W of 0.95 with 2000, one might consider halting the PSA calculation. But the evidence of the Level E exercise is that W might well revert to a relatively low value after further samples (e.g., 3000) were

taken. Thus, the Shapiro-Wilk statistic is too unreliable, for the results presented here, to serve as an indicator that a sufficiently large sample size has been reached for normal confidence intervals to be safely used.

W values and Shapiro-Wilk confidence limits for other time points for I-129, as well as for the Neptunium chain, lead to similar conclusions as those drawn from an analysis of Figs. 3.9 and 3.10. In summary, these results do not support the practice of describing PSA results as converged as soon as W has reached some critical value. It is recommended, therefore, that Chebyshev's Inequality be used to calculate confidence intervals until an improved analysis is found, either one which - like the Chebyshev analysis - is free of assumptions about the underlying distributions (e.g., Woo, 1989), or one which adjusts the interval size according to information about the distributions.

3.4 Sampling-Scheme Efficiency

The discussion in Section 3.3 ignored the possibility that confidence intervals may have been systematically different from one participant to the next, depending on the sampling strategy used. A sampling scheme can be considered more efficient if, for a given sample size, it leads to estimates of mean dose subject to smaller statistical variance. To be useful, however, any such improved efficiency must be supported by quantitatively determined confidence intervals.

3.4.1 LHS versus MC Sampling

All but one of the contributions used either the LHS or MC sampling schemes. Direct comparison between the two schemes is, however, hampered by the lack of any useful formula for the variance of the estimator for mean under LHS, as already noted in Section 3.1. Because LHS results are unsupported by an appropriate confidence-interval analysis, participants using LHS calculated confidence intervals with Eqn. (3.7), just as though MC sampling were in use and the sampled values could be considered as independent. The drawback of this approach is that in LHS, the samples are not independent; rather, they are arranged so that the parameter values more uniformly represent their specified distributions. Indeed, it is precisely this that is supposed to make the variance of the estimator for mean [Eqn. (3.1)] less than with MC sampling.

Thus, because of the approach for deriving confidence intervals with LHS, it is not possible to see a systematic difference in confidence-interval size between the LHS and MC sampling schemes (e.g., Figs. 3.7 to 3.10). The only trend which might be expected is for the actual mean estimates (the centres of the intervals) to be closer to the true mean with LHS than with MC sampling. The number of contributions is, however, insufficient to discern whether such a trend exists.

3.4.2 IS versus MC Sampling

Importance Sampling should lead to reduced variance in mean estimates over MC sampling by adjustment of the parameter sampling distributions, such that the summand in Eqn. (3.2) itself has reduced variance. The variance of the estimator for mean can be calculated using expressions closely analogous

to those for MC sampling [compare Eqns. (3.7) to (3.9)], so that reductions in the size of confidence intervals should be directly observable. In the Level E exercise, only one contributor used IS, and that only for the Neptunium-chain results. Thus, although the confidence intervals found in this case were generally smaller than those obtained using MC sampling with comparable sample sizes, there are insufficient results with IS to conclude reliably what level of reduction in confidence-interval size could normally be expected.

3.5 Radionuclide Ranking

Sensitivity analysis, in which the model parameters are ranked in order of importance, may be the subject of a separate PSACOIN exercise (provisionally known as Level S). Several different techniques are available for conducting such analyses and previous experience has shown the need to define the requirements of such analyses clearly (see NEA PSAC User Group, 1987). On the other hand, the ranking of radionuclides in the order in which they contribute to dose is more easily defined, and has been included here. In addition, exact results are available from the ESCORT code.

Participants were asked to rank the four radionuclides in decreasing importance of contribution to the mean dose at 10 different times, spanning the period 1×10^4 to 1×10^7 a. Radionuclide ranking is normally carried out with a postprocessing code. Thus, this part of the Level E exercise assists in the verification of these postprocessing codes.

The participants' results are summarised in Table 3.1. The exact solutions for the mean dose for the different radionuclides are also given in this Table, as deduced from Figs. 3.11a-b. These figures were produced using the ESCORT code and show the correct ranking in a continuous way over time. For times up to 5×10^4 a, the contribution to mean dose from the Neptunium chain is negligible, and some participants have therefore ranked only Iodine. All participants have provided the correct ranking for this time period.

Immediately after 1×10^5 a, a crossover occurs between U-233 and Th-229 (Figs. 3.11a-b); all participants ranked the nuclides correctly at 1×10^5 a. At 2×10^5 a, the contribution from I-129 crosses that of U-233 and Th-229. Most results continue to show the correct ranking at this time, the few exceptions having ranked U-233 and Th-229 inversely. It should be noted, however, that the contributions from these two nuclides are almost equal at this time.

At 5×10^5, 1×10^6, and 2×10^6 a, the rankings are provided correctly by all participants but one. Crossovers occur again at 1×10^6, 5×10^6, and 1×10^7 a, although the contributions of the nuclides at times greater than 5×10^6 a are nearly equal.

In conclusion, the postprocessing codes used yield excellent agreement with the exact results for all participants but one. With the exception of this participant (at times 5×10^5 to 2×10^6 a), all discrepancies are minor, occurring between two nuclides whose contributions to dose are relatively small and very nearly equal. This part of the Level E exercise has contributed, therefore, to the verification of these postprocessing codes.

3.6 Principal Component Analysis

As in Section 2.2 for the deterministic results, a global analysis of the stochastic results provided by the participants was carried out by PCA. Figure 3.12 shows projections of the participants' results for all deterministic and some stochastic parameters, for all radionuclides considered, onto the first two principal component axes. These two principal components describe 54% of the variance of the 71 variables considered. Figure 3.13 is similar to Fig. 3.12 except that only the 17 I-129 variables are considered. Because PCA cannot accomodate participants providing incomplete results, this subset of the data allows results from those participants that completed only the I-129 part of the Level E questionnaire to be considered in the global analysis.

The exact results are labelled with the letter A in Figs. 3.12-3.13. Both PCA plots provide evidence of discrepancies similar to those observed in Fig. 2.9. In addition, the results of the same participants - where available - tend to be discrepant in all these figures. This analysis confirms, therefore, that a few participants have provided results deviating from either the exact or the "average" results (or both). In addition, the analysis shows that the majority of the participants' results agree reasonably well.

Fig. 3.1 Mean dose from I-129 at six times, and exact solution (continuous line).

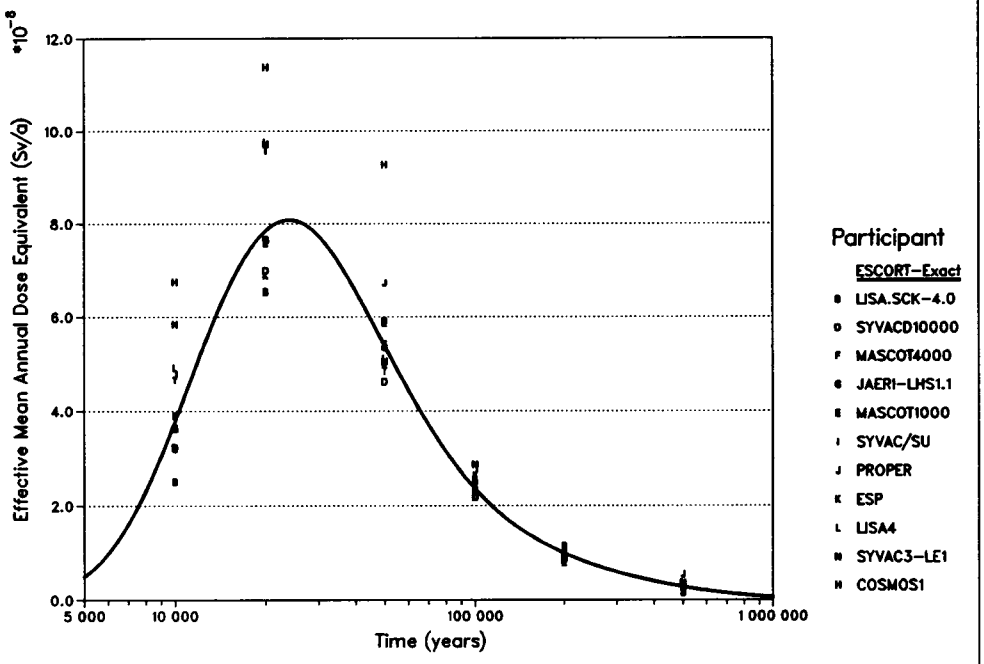


Fig. 3.2 Mean total dose from Neptunium chain at five times, and exact solution (continuous line).

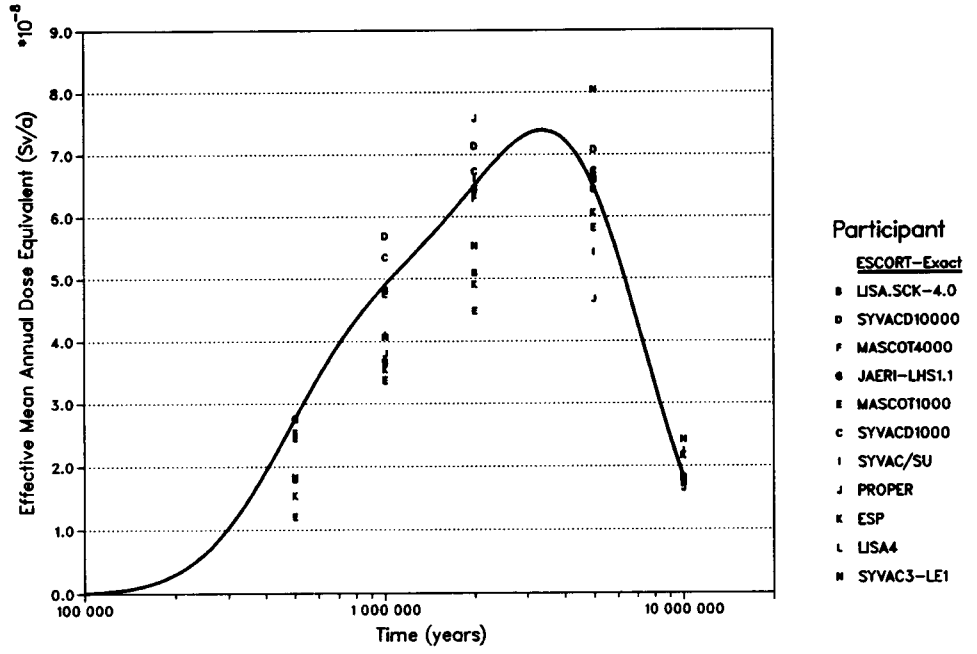


Fig. 3.3 Mean values of maximum dose up to six given times from I-129.

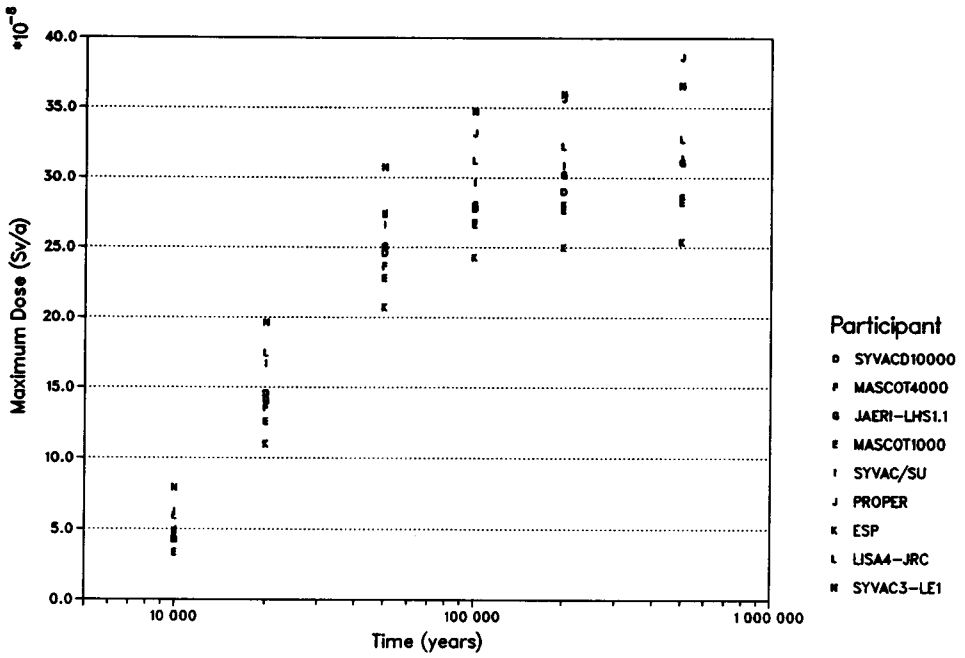


Fig. 3.4 Mean values of maximum total dose up to five given times from the Neptunium chain.

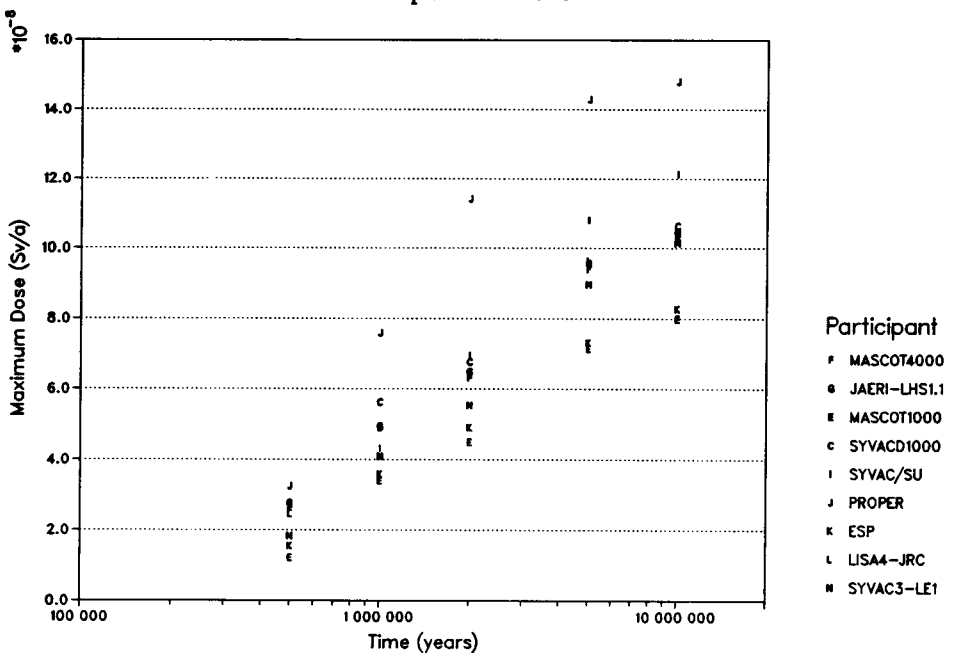


Fig. 3.5 Standard deviation of the mean dose from I-129 at six times.

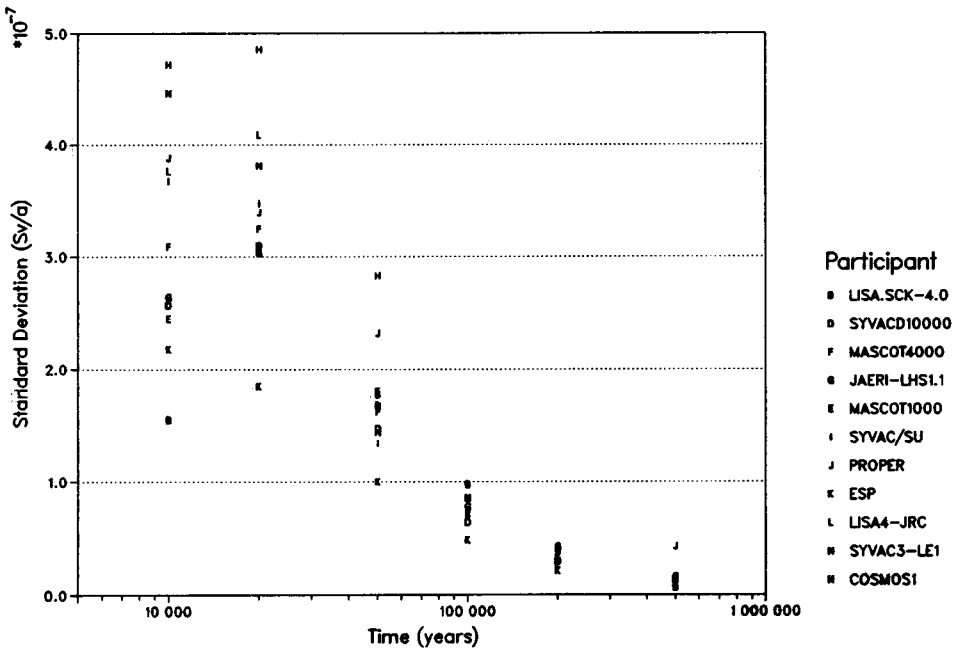


Fig. 3.6 Standard deviation of the mean total dose from the Neptunium chain at five times.

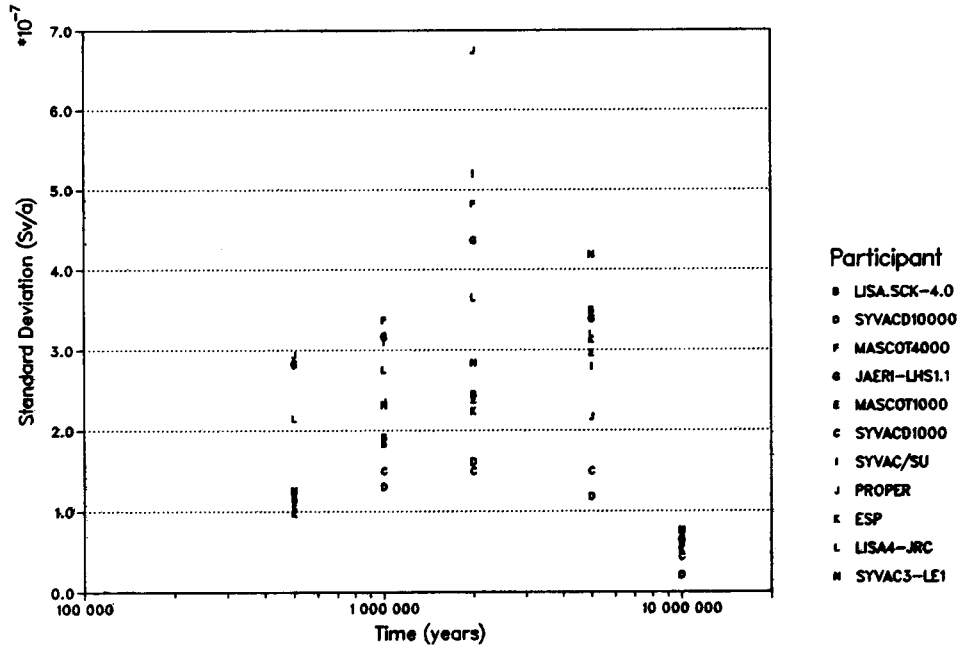


Fig. 3.7 Chebyshev confidence intervals for the mean dose from I-129 at 2 x 10^4 a, versus $N^{-½}$ (N is sample size).

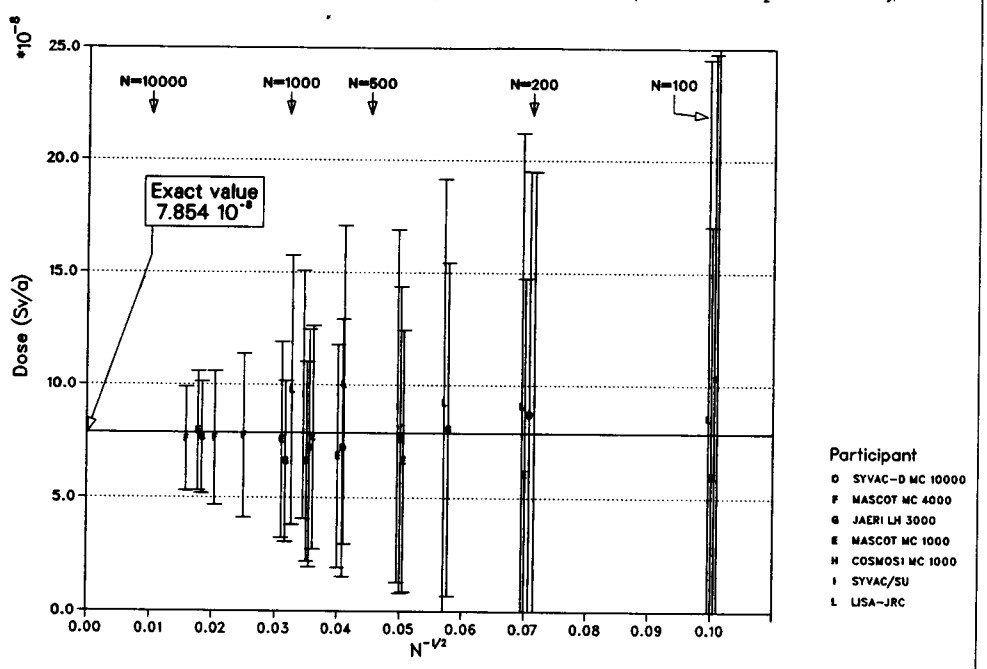


Fig. 3.8 Chebyshev confidence intervals for the mean total dose from the Neptunium chain at 2 x 10^6 a, versus $N^{-½}$ (N is sample size).

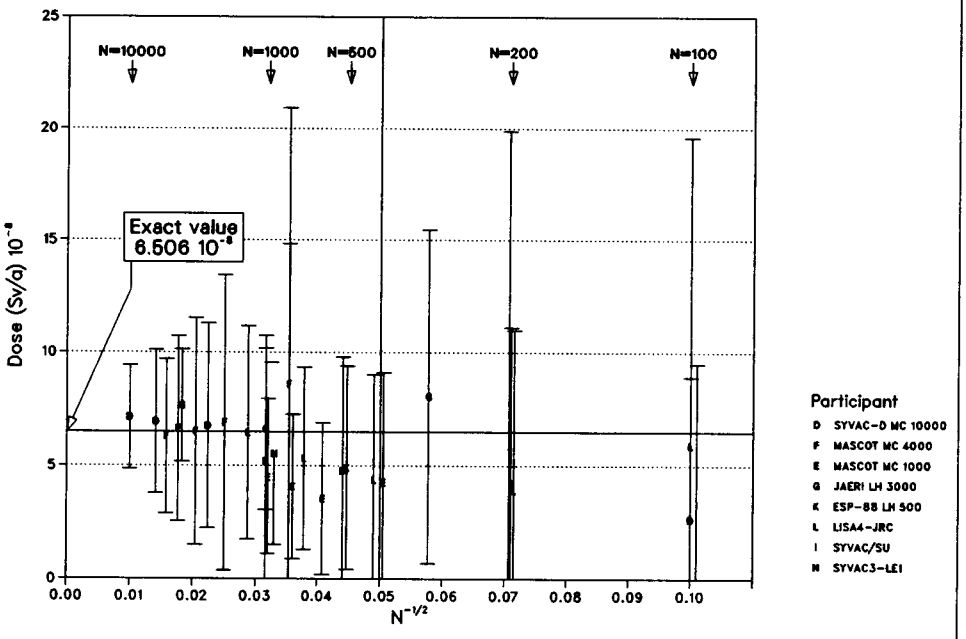


Fig. 3.9 Shapiro-Wilk test statistic, W, for the dose from I-129 at 2 x 10^4 a, versus $N^{-½}$ (N is sample size).

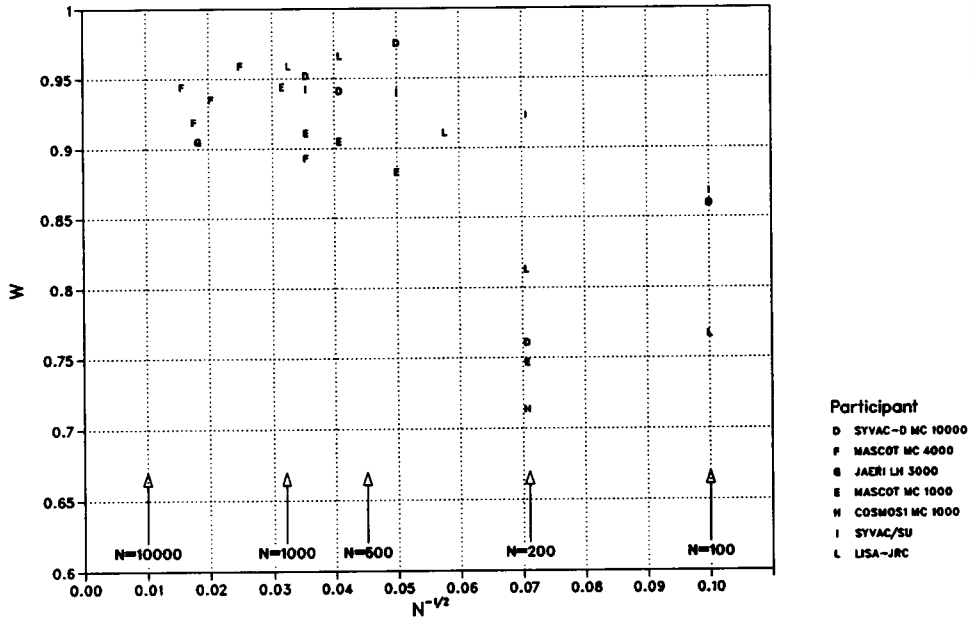


Fig. 3.10 Shapiro-Wilk confidence intervals for the mean dose from I-129 at 2 x 10^4 a, versus $N^{-½}$ (N is sample size).

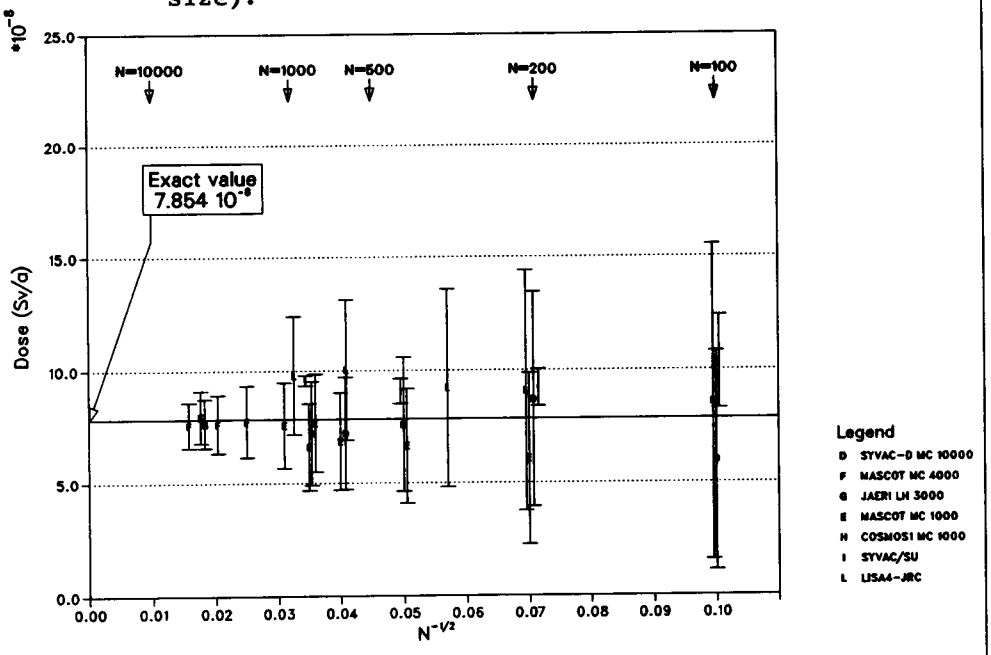


Fig. 3.11a PSACOIN Level E exact doses versus time from I-129, Np-237, Th-229, U-233, and the sum thereof, plotted on a linear-log scale.

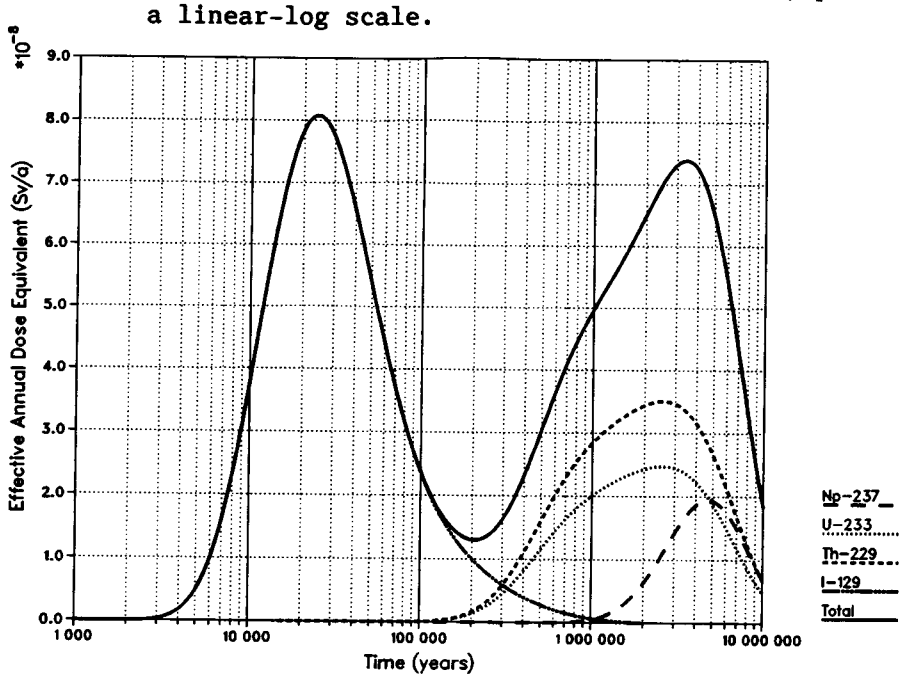


Fig. 3.11b PSACOIN Level E exact doses versus time from I-129, Np-237, Th-229, U-233, and the sum thereof, plotted on a log-log scale.

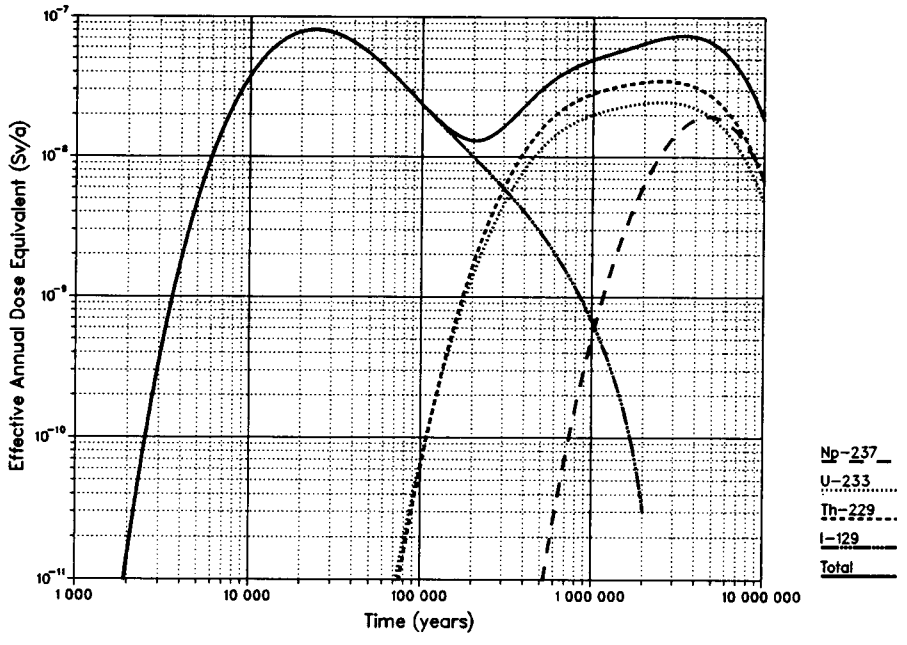


Table 3.1 PSACOIN Level E ranked contributors to mean dose.

Participant / Time		Method	10^4	$2 \cdot 10^4$	$5 \cdot 10^4$	10^5	$2 \cdot 10^5$	$5 \cdot 10^5$	10^6	$2 \cdot 10^6$	$5 \cdot 10^6$	10^7
CEN/SCK	200	LH	I	I	I	IUT	ITU	TUI	TUIN	TUNI	TNU	TNU
NRPB	500	LH	IUTN	IUTN	IUTN	IUTN	ITUN	TUIN	TUIN	TUNI	TUNI	TNUI
JAERI	3000	LH	IUTN	IUTN	IUTN	IUTN	IUTN	TUIN	TUIN	TUNI	TUNI	NTUI
PNC	100	LH	I	I	ITUN	ITUN	ITUN	TUIN	TUNI	TUNI	TUNI	TNUI
AERE-H	1000	MC	IUTN	IUTN	IUTN	IUTN	IUTN	TUIN	TUIN	TUNI	TUNI	NTUI
AERE-H	4000	MC	IUTN	IUTN	IUTN	IUTN	ITUN	TUIN	TUIN	TUNI	TNUI	NTUI
SKI	800	MC	I	IUTN	IUTN	IUTN	IUTN	UTIN	UTNI	UTNI	TUNI	NTUI
UKDOE	10000	MC	IUTN	IUTN	IUTN	IUTN	IUTN	TUIN	TUIN	TUNI	TUNI	NTUI
AECL/WNRE	1000	MC	ITUN	ITUN	IUTN	IUTN	ITUN	TUIN	TUIN	TUNI	TNUI	TNUI
INTERA		Exact	IUTN	IUTN	IUTN	IUTN	ITUN	TUIN	TUIN	TUNI	TNUI	NTUI

Sampling Methods: MC Monte Carlo, IS Importance Sampling, LH Latin Hypercube

$I \longrightarrow I^{129}$, $N \longrightarrow Np^{237}$, $T \longrightarrow Th^{229}$, $U \longrightarrow U^{233}$

Fig. 3.12 PCA for all output variables (deterministic and stochastic) for which the exact solution is available, showing the first (31%) and second (23%) principal components. Note that participants C, D, H and K are not included because they did not submit complete sets of results (see Sections 2.2 and 3.6 for explanation).

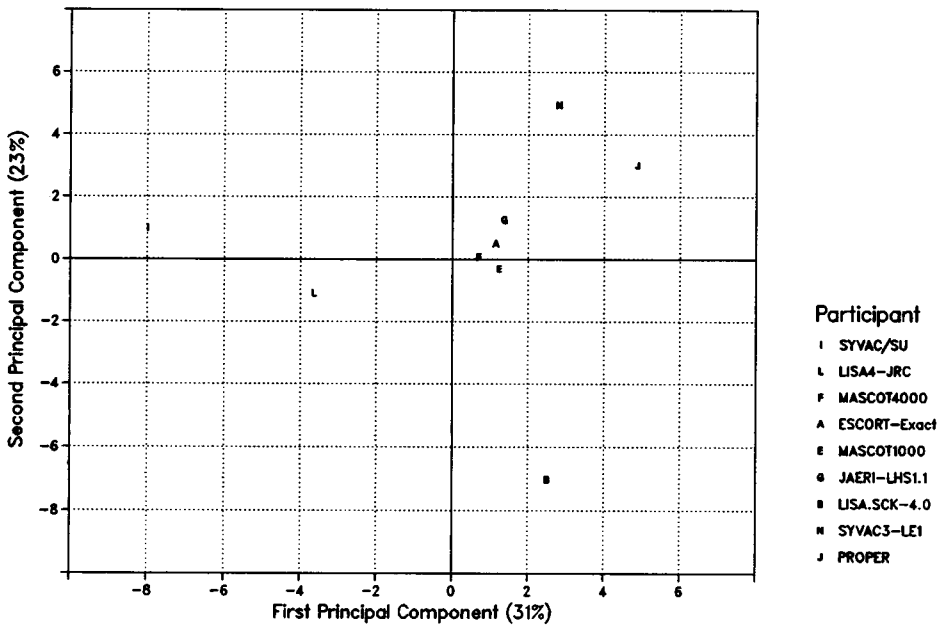
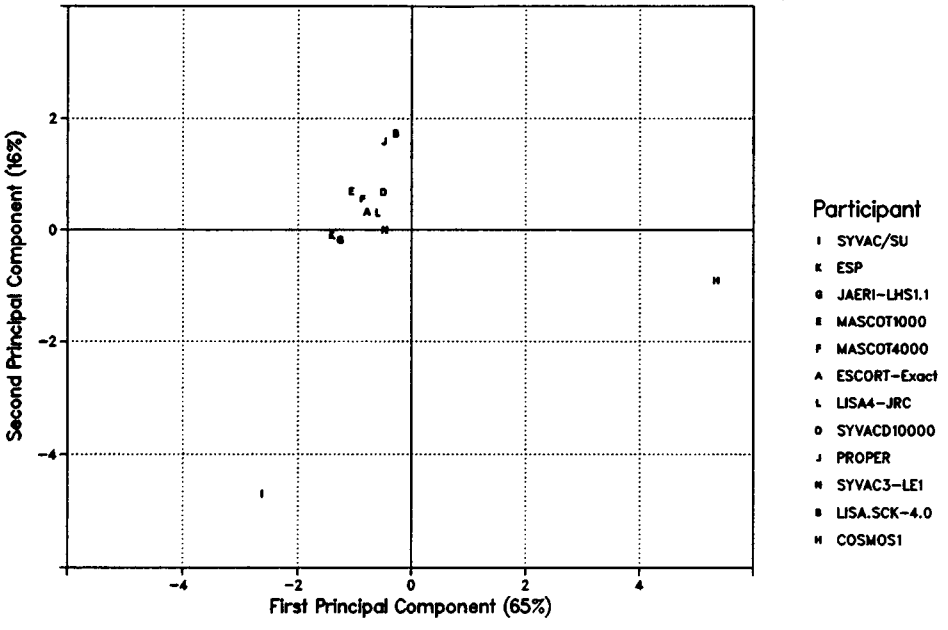


Fig. 3.13 PCA for all I-129 output variables (deterministic and stochastic) for which the exact solution is available, showing the first (65%) and second (16%) principal components (see Sections 2.2 and 3.6 for explanation).



4. CONCLUSIONS AND RECOMMENDATIONS

The PSACOIN Level E exercise has contributed substantially to the verification of PSA codes for assessments of radioactive waste disposal systems. In terms of the four objectives of the Level E intercomparison, the following specific conclusions can be drawn and recommendations made.

(1) The results from the 10 participating codes show a high degree of consistency for both deterministic and stochastic analyses, despite the use of different codes, sampling schemes, and sampling sizes. Such agreement contributes to the verification of the executive portion of PSA codes, as well as those submodels that might eventually be used in formal safety assessment studies.

(2) Results from most of the PSA codes also agree well with the exact solution. In one situation, a tendency was found for the PSA codes to agree better with each other than with the exact solution - specifically, there was a tendency to underestimate mean dose. This situation is thought likely to arise only at early times when the mean dose is far below its peak value. In principle, this problem can be avoided by taking larger sample sizes.

(3a) The exercise was unable to demonstrate any difference in efficiency between Latin Hypercube Sampling (LHS) and Monte Carlo (MC) sampling with regard to convergence of sample means. Further research is required to evaluate the relative efficiencies of the two methods in PSA applications typical for radioactive waste disposal systems.

(3b) Only one participant employed the Importance Sampling strategy. Because of the design of the Level E case, however, the value of this strategy was inadequately tested. A more complex case is required to evaluate the relative efficiencies of the two methods.

(3c) An additional conclusion is that confidence intervals for estimated mean values based on Chebyshev's Inequality are reliably conservative, whereas the so-called "normal" confidence intervals, as supported by the Shapiro-Wilk test, are less reliable. The latter confidence intervals were shown in practice to be frequently too narrow - particularly with small sample sizes - based on a comparison of these intervals with the exact solution. An improved method for providing distribution-free confidence intervals, however, using Guttman's Inequality, has recently been discovered (Woo, 1989).

(4) The source-term and geosphere components of the system model are similar to submodels currently in use by many of the participants and may eventually be used in formal safety assessment studies by some of these participants. The Level E exercise has substantially contributed to the verification of the code for these submodels.

Several more general recommendations can be added.

(5) Most importantly, it is recommended that further code intercomparisons be pursued, with greater emphasis on the use of system models that are more representative of specific concepts for the disposal of radioactive waste.

(6) With regard to questionnaires for future PSACOIN exercises, it is recommended that these elicit plots for deterministic runs of consequence (e.g., dose) versus time, in a well-defined format, as an aid during preliminary comparison of the quality of results, particularly for comparisons involving complex system models. In addition, if large volumes of data are to be elicited (close to 600 per participant for the Level E exercise), these should be transferred to the NEA Data Bank preferably in machine-readable form, and not only by paper.

(7) With regard to the mechanical part of the intercomparison, PSA code verification exercises of this kind were found to benefit particularly from the inclusion of several deterministic runs, principal component analysis of both deterministic and stochastic results, plots of mean dose at specified times, and nuclide rankings. Data on dose distribution, although elicited in the questionnaire, were not discussed in the report because comparisons of histograms and downward cumulative distribution curves were not found to add additional insight. Finally, parameter ranking was not addressed in this study, and is still considered a useful but particularly difficult exercise to define.

ANNEX A

PSACOIN Level E Intercomparison Case Specification and Results Elicitation Form containing Tables of Exact Results

This Annex is a reproduction of PSAC/DOC(87)13. This document was prepared by S. Oldfield, J. Sinclair, T. Andres, and P. Robinson. Appendix 3 of this Annex, "Graphical Presentation of Reference Results", has not been reproduced here, however, because similar graphs can be found in the main body of the report.

Note that parts C5 and C6 of the questionnaire elicit dose distributions at given times. These data were not discussed in the main body of the report because they were not found to add additional insight, although histograms and downward cumulative distribution curves were compared.

C O N T E N T S

1. Introduction

The NEA Probabilistic System Assessment Code (PSAC) User Group is conducting a series of international comparisons for computer codes which use the PSA approach to model radionuclide migration from underground disposal of radioactive wastes. These tests help to build confidence in the correct functioning of PSA codes, and in their ability to adequately represent the waste disposal systems being modelled. The title of the intercomparison series is PSACOIN. This document provides the specification for the 'Level E' case study, which is intended to be complementary to, and extend, the Level 0 intercomparison already reported [1].

The Level E case study is based on models of radionuclide release and migration which are simple, but somewhat more realistic than those used in Level 0. The most important feature of the new case, however, is that the models are chosen to allow exact calculation of the mean dose rates (hence E for Exact in the title). Thus the PSA code results — estimates of mean dose rates based on finite samples from the space of model parameters — can be compared not only with each other, but also with the exact results which effectively correspond to an infinite sample size.

The 'exact' results arise from analytic expressions for integrals over parameter space of the model dose rate, expressed as a Laplace transform rather than as a function of time. These integrals are tractable only for certain simple choices of the probability distribution functions (PDFs) for the model parameters. A report by Robinson and Hodgkinson [2] describes the general approach, and explains how a high-precision Laplace transform inversion technique allows the results to be calculated to a precision approaching that of the computer used. Not included in that report are recent extensions to handling decay chains. A computer program, ESCORT, is available which has been used for computing the reference results for the present case study, and can be used for other similar modelling. A version of ESCORT, based on the original of Peter Robinson, has been prepared for the UK DoE by CAP Scientific Ltd. It is expected that this will be made widely available through the NEA Data Bank.

Within the limits imposed by the available analytic solutions, the Level E case specification is designed to represent a hypothetical deep land disposal facility. The repository itself is represented by a simple leach-rate controlled release of radionuclides into the groundwater of a host rock. The radionuclides are transported through two geosphere layers with different hydrogeological properties. Thence, contamination is assumed to enter a stream from which the critical group obtains drinking water. This model of the transport process and exposure pathway to Man is fully described in Appendix 1.

The objectives of the PSACOIN Level E exercise can be stated as:

(i) To demonstrate the correct operation of PSA code 'executive' functions, such as input, output, internal data transfers, random number generation, and statistical post-processing.

(ii) To gain further experience in the specification, coding, and comparison of PSA codes.

(iii) To compare PSA code results against a known solution.

(iv) To provide a case study with sufficient similarity to practical assessment requirements that production sub-model codes can be used, rather than special modules written for the purpose of the exercise.

(v) To provide a common basis for assessing the relative efficiencies of different parameter sampling schemes.

Objectives (i) and (ii) applied also to the the Level 0 exercise, while (iii) is of course unique to Level E. Regarding objective (iv), it is recognised that almost any existing code may well require minor modification or extension to enable the case specification to be adequately represented, or to provide results in the common form laid down. However, it is hoped that in most cases, existing radionuclide release and migration sub-models will be usable. Where this is so, the exercise is obviously more valuable as part of the quality assurance of participant's codes.

To aid in assessing the suitability of particular code modules, and in checking their implementation, several sets of deterministic results are provided, obtained by using ESCORT with all parameters fixed. These include not only final dose values, but also intermediate outputs from the source and first geosphere sub-models. Although the Questionnaire for submitting code results (Appendix 2) provides for these deterministic results to be entered, it is primarily the participants' responsibility to ensure adequate correspondence with the reference results.

To conduct an effective intercomparison of probabilistic results, it is necessary that all participants sample parameter values from the PDFs laid down, and return the particular statistical descriptions of their results requested on the Questionnaire. Within the limits of this basic degree of standardisation, there is freedom for participants to employ a variety of methods. This gives a considerable scope for confusion. For instance, one sampling scheme may inherently give rise to a smaller variance in its sampled results than another. Despite this, different methods should give similar estimates of the variance of the underlying dose distribution. What should differ is the degree of uncertainty in the estimates of the mean (or other statistics). In other words, one method may give rise to smaller confidence intervals than another. To help avoid misunderstandings, Section 3 of this document aims to make as explicit as possible the meaning of each requested quantity, and to spell out where variety of method is welcomed.

Clearly, there is expected to be some scatter among nominally equivalent statistical results when finite sample sizes are used. Although the exact reference values are being made freely available, participants are asked to avoid any selection of results for submission according to their agreement with the reference values. For instance, a 95% confidence interval for any given estimated quantity would be expected to exclude the 'true' answer about once in every 20 independent trials, and it would distort the intercomparison if anyone were to try again with a different random number seed, just to avoid such a discrepancy.

This case specification has been prepared by the coordinating panel listed below. Queries may be addressed to any of us.

Steve Oldfield†	Electrowatt Engineering Services (UK) Ltd., Grandford House, 16 Carfax, Horsham, W. Sussex, RH12 1UP England
Jim Sinclair	Theoretical Physics Division, UKAEA Harwell Laboratory, Harwell, Oxfordshire, OX11 0RA England
Terry Andres	AECL Whiteshell Nuclear Research Establishment, Pinawa, Manitoba, R0E 1L0 Canada
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†Steve has now left Electrowatt, and Jean–Marc Laurens has taken over his work as coordinator of the Level–E exercise.

2. Case Specification

2.1 The Model

The model chosen for the intercomparison is fully described in Appendix 1. It contains four sub-models: a source term, two geosphere layers, and a biosphere. Four nuclides are considered: I–129, and the chain Np–237, U–233, Th–229. The model has 33 parameters, 21 of which always take fixed values, while 12 are taken as random variables (except in the deterministic test cases).

A feature of the model which may be difficult for some PSA codes to implement is the nature of the boundary conditions at the downstream end of the geosphere layers (see equations A1.8, A1.10). Specifying conditions 'at infinity' was necessary in order to make the integrals in the exact solution tractable. With many numerical solution techniques, it may be more convenient to require continuity of concentration and flux and the boundary between the two layers. Such a discrepancy with the specified model will probably be acceptable. Trials [3] suggest that the results will be rather insensitive to the choice of boundary conditions at the end of layer 1.

The fundamental output of the model is an annual effective dose equivalent as a function of time, which we call simply 'dose' in the following. The dose contributions $D_i(t)$ arising from different nuclides can be separated; we shall write the contribution from I–129 as $D_I(t)$, and the total contribution from the Np–237 chain as $D_C(t)$. It is sometimes convenient to show explicitly the dependence on the model parameters, by writing e.g. $D_I(t; \mathbf{p})$, where the vector $\mathbf{p}$ is a collective representation of all the parameters.

2.2 Fixed Parameter Cases

Although the main purpose of the exercise is to compare probabilistic dose results, it is useful for checking individual codes to have available reference results for several 'deterministic' cases, i.e. with all parameters fixed. Three fixed cases have therefore been chosen, with parameter values as shown in Table 1, in the columns headed 'deterministic cases'. The reference results obtained using ESCORT are included in the Questionnaire (Appendix 2). Appendix 3 presents the results graphically, showing more clearly the way the sub-model outputs vary with time. Full tables of the results in numerical form are available on request from Jim Sinclair.

2.3 Varying Parameter Cases

Table 1 shows the chosen PDFs for the 12 variable parameters, and the fixed values of the others. Note that the choice of PDFs is somewhat limited by the exact integration formulae available; for instance, choice of normal distributions would have made the integrations intractable. Again, the reference results are included in the Questionnaire, and Appendix 3 shows graphically the expectation value of dose contributions versus time.

3. Quantities to be Compared

The exact results available from ESCORT are expectation values of the dose as a function of time:

$$E(D_i(t)) \equiv \int_{\mathbf{p}} D_i(t; \mathbf{p})\, f(\mathbf{p})\, d\mathbf{p}. \tag{3.1}$$

Here, $f(\mathbf{p})$ is the joint PDF for the parameters. Since they are independent, it is simply the product of the 12 individual PDFs.

Each PSA code will produce **estimates** of $E(D_i(t))$, based on a finite number of simulations with sampled parameter values. We shall use a circumflex notation to denote such estimated quantities, e.g. $\hat{E}(D_i(t))$. In the case of simple Monte Carlo sampling, the estimator for the expectation value will be a simple average:

$$\hat{E}(D_i(t)) \equiv \frac{1}{N} \sum_{n=1}^{N} D_i(t; \mathbf{p}_n), \tag{3.2}$$

where $\mathbf{p}_n$, $n = 1...N$ are the sampled parameter sets. With other strategies, such as importance sampling, different expressions may be required.

A PSA code can also produce a number of other statistics for which no exact value is available for comparison. For instance, the maximum of dose up to a certain time,

$$P_i(t) \equiv \max_{t' \leq t} D_i(t'), \tag{3.3}$$

can be averaged. More importantly, the variability among sampled results can be used to estimate the true variance of the model results. For instance, from simple Monte Carlo sampled results, an estimator for the variance of dose is

$$\hat{\sigma}^2(D_i(t)) = \frac{1}{N-1} \sum_{n=1}^{N} \left[D_i(t; \mathbf{p}_n) - \hat{E}(D_i(t))\right]^2. \tag{3.4}$$

Other sampling schemes will give rise to different formulae.

Further types of code results which are interesting to compare include histograms of the distribution of dose, and the way the statistical quantities produced by the codes vary with the number of runs used. In the Questionnaire (Appendix 2), results of all the above types are requested.

3.1 Confidence Limits

It is clearly important to be able to set soundly based confidence bounds for estimated mean doses or risks produced by PSA codes. However, no consensus appears to exist as to how this should be done. In this exercise, therefore, participants are asked to apply two particular methods, and also to submit alternative measures based on other schemes of their own choice.

The major source of difficulty in setting confidence bounds in waste disposal applications is the extreme skewness usually found in the dose distributions. The usual assumption that the mean of a 'large' sample is a normally distributed statistic may consequently be invalid. The two approaches suggested below are based on either assuming nothing about the distribution of the mean, or on the other hand establishing normality before proceeding.

3.1.1 Use of Chebyshev's Inequality

For any random variate y with finite standard deviation σ and mean μ, the probability of a sample deviating from μ by more than a given multiple of σ is bounded, according to Chebyshev's inequality, by

$$P(|y - \mu| \geq r\sigma) \leq 1/r^2. \tag{3.5}$$

This holds whatever the shape of the distribution of y, and therefore looks at first sight to be the basis of establishing confidence intervals for a mean which are guaranteed to be conservative. However, it is worth noting that σ is usually not known *a priori*, so if an estimate, $\hat{\sigma}$, is substituted, the bound may become non-conservative. This is a particular danger in the present type of application, where a modest-size sample of dose results may omit rare large values, and consequently not only underestimate the mean, but grossly underestimate the variance of dose.

With these cautions borne in mind, Chebyshev's Inequality provides the basis for assigning as a 95% confidence interval for mean dose

$$\hat{E}(D_i(t)) \pm 4.47\, \hat{\sigma}(D_i(t)) / \sqrt{N}. \tag{3.6}$$

As for equations (3.2) and (3.4), this formula applies only to simple Monte Carlo sampling, where $\hat{\sigma}(D_i(t)) / \sqrt{N}$ is an estimator for the standard error in the estimate (3.2) of the mean dose. Other sampling schemes, in which the mean dose is estimated via quantities of lower variance, may be able to provide tighter confidence intervals on the basis of Chebyshev's inequality.

3.1.2 Use of Normality Tests on the Mean

Given (say) 1000 dose values (obtained by random sampling of model parameters), it is clearly impossible to test the normality of the distribution of the means of all possible samples of this size. Instead, the 1000 may be divided into a number of batches, and the distribution of the batch means tested. If this proves to be close to normal, it is reasonable to assume that the mean over 1000 values would be even closer to normal. It is proposed that participants whose sampling schemes are suitable should follow such a procedure, as a further route to setting confidence intervals on mean dose values. Those who use Latin Hypercube Sampling, or any other experimental design in which the samples are not independent, will only be able to follow this route if they are willing to apply their sampling scheme to each batch independently.

Suppose M equal batches are taken, yielding means B_m. It is required to test the hypothesis that the B_m are drawn from a normal distribution. A commonly used test for this purpose is Shapiro–Wilk's W–test [4,5]. The W–statistic is computed as follows:

1) Order the batch means so that

$$B_1 \leq B_2 \leq \ldots \leq B_M.$$

2) Calculate the mean $\bar{B}$ and the sum of square deviations

$$S^2 = \Sigma_m (B_m - \bar{B})^2.$$

3) Finally calculate

$$W = \left(\Sigma_m a_m B_m\right)^2 / S^2, \tag{3.7}$$

using tabulated coefficients a_m (these depend on M).

The value of W must lie between zero and one. In general, small W values imply that the B_m are very unlikely to be drawn from a normal distribution, but the distribution function for W also depends on the number of batches. With $M = 10$, for example, a W–value less than 0.897 should only occur with 20% probability, with samples that do come from a normal distribution. Hence, a test result of $W = 0.897$ would indicate normality at only 20% significance level.

It is important not to confuse the significance level used in judging the normality of the means with that used in the confidence interval placed on the mean of the underlying dose distribution. Probably it would be sufficient to establish normality with 50% confidence, but participants are free to set their own standards, indicating in the Questionnaire what they have done. For cases where the batch means are accepted as being normally distributed, the 95% confidence interval for mean dose becomes

$$\hat{E}(D_i(t)) \pm 1.96\, \hat{\sigma}(Q) / \sqrt{N}, \tag{3.8}$$

with interpretation and restriction just as for equation (3.6). Note that at this stage, the full sample size N may be used, not the batch size N/M.

Table 2 gives the coefficients a_m to be used in equation (3.7) when the number of batches, M, is 10. Table 3 gives the W values associated with a variety of significance levels for the normality test. For corresponding data for other M values, see for instance Hahn and Shapiro [5].

References

[1] Nuclear Energy Agency, *PSACOIN Level 0 Intercomparison,* Paris: OECD, 1987.

[2] P.C. Robinson and D.P. Hodgkinson, Exact solutions for radionuclide transport in the presence of parameter uncertainty, *Radioactive Waste Management and the Nuclear Fuel Cycle,* **8**(4), 283–311 (1987).

[3] P.C. Robinson, informal presentation to 6th PSAC meeting, Paris, December 1987.

[4] S.S. Shapiro and M.B. Wilk, An analysis of variance test for normality (complete samples), *Biometrika* **52**, 591–611 (1965).

[5] G.J. Hahn and S.S. Shapiro, *Statistical Models in Engineering,* New York: Wiley, 1967.

Table 1 Parameter values and ranges

Parameter	Probabilistic case		Deterministic cases			Units
	PDF type	Values	Fixed 1	Fixed 2	Fixed 3	
$M_I^{(0)}$	fixed	100	100	100	100	mols
$M_N^{(0)}$	fixed	1000	1000	1000	1000	mols
$M_U^{(0)}$	fixed	100	100	100	100	mols
$M_T^{(0)}$	fixed	1000	1000	1000	1000	mols
λ_I	fixed	4.41×10^{-8}	4.41×10^{-8}	4.41×10^{-8}	4.41×10^{-8}	yr^{-1}
λ_N	fixed	3.24×10^{-7}	3.24×10^{-7}	3.24×10^{-7}	3.24×10^{-7}	yr^{-1}
λ_U	fixed	4.37×10^{-6}	4.37×10^{-6}	4.37×10^{-6}	4.37×10^{-6}	yr^{-1}
λ_T	fixed	9.44×10^{-5}	9.44×10^{-5}	9.44×10^{-5}	9.44×10^{-5}	yr^{-1}
T	uniform	100 to 1000	100	300	1000	years
k_I	log-uniform	10^{-3} to 10^{-2}	10^{-2}	3×10^{-3}	10^{-3}	yr^{-1}
k_C	log-uniform	10^{-6} to 10^{-5}	10^{-5}	3×10^{-6}	10^{-6}	yr^{-1}
$v^{(1)}$	log-uniform	10^{-3} to 10^{-1}	10^{-1}	5×10^{-2}	3×10^{-2}	m yr^{-1}
$l^{(1)}$	uniform	100 to 500	100	200	500	metres
$d^{(1)}$	fixed	10	10	10	10	metres
$R_I^{(1)}$	uniform	1 to 5	1	3	3	–
$R_{0N}^{(1)}$	fixed	100	100	100	100	–
$R_{0U}^{(1)}$	fixed	10	10	10	10	–
$R_{0T}^{(1)}$	fixed	100	100	100	100	–
$\gamma_C^{(1)}$	uniform	3 to 30	3	5	8	–
$v^{(2)}$	log-uniform	10^{-2} to 10^{-1}	10^{-1}	3×10^{-2}	10^{-2}	m yr^{-1}
$l^{(2)}$	uniform	50 to 200	50	100	200	metres
$d^{(2)}$	fixed	5	5	5	5	metres
$R_I^{(2)}$	uniform	1 to 5	1	3	3	–
$R_{0N}^{(2)}$	fixed	100	100	100	100	–
$R_{0U}^{(2)}$	fixed	10	10	10	10	–
$R_{0T}^{(2)}$	fixed	100	100	100	100	–
$\gamma_C^{(2)}$	uniform	3 to 30	3	10	8	–
w	fixed	0.73	0.73	0.73	0.73	$m^3\ yr^{-1}$
W	log-uniform	10^5 to 10^7	3×10^5	10^6	3×10^6	$m^3\ yr^{-1}$
β_I	fixed	56	56	56	56	Sv mol^{-1}
β_N	fixed	6800	6800	6800	6800	Sv mol^{-1}
β_U	fixed	5900	5900	5900	5900	Sv mol^{-1}
β_T	fixed	1.8×10^6	1.8×10^6	1.8×10^6	1.8×10^6	Sv mol^{-1}

Table 2 Coefficients a_m used in W test for normality, for $M = 10$

$-a_1$ $= a_{10}$	$-a_2$ $= a_9$	$-a_3$ $= a_8$	$-a_4$ $= a_7$	$-a_5$ $= a_6$
0.5739	0.3291	0.2141	0.1224	0.0399

Table 3 Significant values of W, for $M = 10$

P is the probability of obtaining a W value as low as that given, by applying equation (3.7) to 10 values B_m actually drawn from a normal distribution.

P	W
1%	0.781
2%	0.806
5%	0.842
10%	0.869
20%	0.897
50%	0.938
80%	0.963
90%	0.972
95%	0.978
98%	0.983
99%	0.986

Glossary of Symbols

The following list gives the meaning of the symbols used throughout the document for parameters, subscripts, superscripts, and operators.

$C_i(x, t)$ concentration (amount per unit length in the transport direction) of nuclide i in the geosphere at position x and time t (mols/m)

d dispersion length in geosphere (metres)

$D_i(t)$ dose (annual effective dose equivalent) arising from nuclide i through drinking water at time t (Sv/yr)

$f(\mathbf{p})$ joint probability density function for the model parameters $\mathbf{p}$

$F_i(x, t)$ flux (amount transported per unit time) of nuclide i in the geosphere at position x and time t (mols/yr)

$G_i(t)$ flux of nuclide i leaving the geosphere at time t (mols/yr)

k leach rate once the containment fails (yr^{-1})

l length of geosphere layer (metres)

M_i amount of nuclide i in the repository at a given time (mols)

$\mathbf{p}$ all the model parameters, considered as a vector

$P_i(t)$ peak dose from nuclide i up to time t (Sv/yr)

Q quantity equal or related to a dose value, obtained from a model calculation with a particular choice of parameter values, which is averaged over the sample calculations to give an estimate of the mean dose.

R_i retardation coefficient for nuclide i (dimensionless)

R_{0i} base retardation coefficient for nuclide i (dimensionless)

$S_i(t)$ flux of nuclide i from the repository at time t (mols/yr)

t time (years)

T containment time during which no leakage occurs (years)

v water travel velocity in geosphere ($\mathrm{m\ yr}^{-1}$)

w individual drinking water requirement ($\mathrm{m}^3\mathrm{yr}^{-1}$)

W (i) stream flow rate ($\mathrm{m}^3\mathrm{yr}^{-1}$)
(ii) Shapiro–Wilk test statistic for normality

x distance from start of geosphere layer (metres)

β dose conversion factor ($\mathrm{Sv\ mol}^{-1}$)

γ_i factor multiplying base retardation coefficient for nuclide i (dimensionless)

λ_i decay constant for nuclide i (yr^{-1})

Subscripts

C denotes the chain Np–237, U–233, Th–229

i denotes nuclide i

I denotes I–129

N denotes Np–237

T denotes Th–229

U denotes U–233

Superscripts

(0) denotes initial value of amount of a nuclide

(1) denotes geosphere layer 1

(2) denotes geosphere layer 2

(k) denotes geosphere layer k (1 or 2)

Operators

$E(y)$ denotes expectation value of a random variable y

$\sigma(y)$ denotes standard deviation of a random variable y

$\hat{y}$ denotes an estimated value of a statistic y

Appendix 1: Mathematical Description of the Model

The test-case model has four sub-models: a source term, two geosphere layers and a biosphere. Four nuclides are considered: I–129 and the Np–237, U–233, Th–229 chain. In the following description the suffices I, N, U and T respectively are used for these nuclides. A suffix C indicates the whole of the chain and a suffix *i* indicates any nuclide.

A1.1 The source term

The source term sub-model consists simply of a delay for an initial containment time, T, followed by leaching at a constant fractional rate. *For the chain, each nuclide has the same leach rate.* To be specific the governing equations are

$$\left.\begin{aligned} \frac{dM_I}{dt} &= -\lambda_I M_I \\ \frac{dM_N}{dt} &= -\lambda_N M_N \\ \frac{dM_U}{dt} &= -\lambda_U M_U + \lambda_N M_N \\ \frac{dM_T}{dt} &= -\lambda_T M_T + \lambda_U M_U \end{aligned}\right\} \quad t < T \qquad \text{(A1.1)}$$

and

$$\left.\begin{aligned} \frac{dM_I}{dt} &= -\lambda_I M_I - k_I M_I \\ \frac{dM_N}{dt} &= -\lambda_N M_N - k_C M_N \\ \frac{dM_U}{dt} &= -\lambda_U M_U + \lambda_N M_N - k_C M_U \\ \frac{dM_T}{dt} &= -\lambda_T M_T + \lambda_U M_U - k_C M_T \end{aligned}\right\} \quad t \geqslant T \qquad \text{(A1.2)}$$

where $M_i(t)$ is the molar amount of nuclide i in the repository at time t. A full list of symbols and units is given on page 11.

The initial conditions are simply

$$M_i(0) = M_i^{(0)} \quad i = \mathrm{I, N, U, T.} \tag{A1.3}$$

The fluxes from the repository are then given by

$$\left.\begin{aligned} S_{\mathrm{I}}(t) &= k_{\mathrm{I}} M_{\mathrm{I}}(t) \\ S_{\mathrm{N}}(t) &= k_{\mathrm{C}} M_{\mathrm{N}}(t) \\ S_{\mathrm{U}}(t) &= k_{\mathrm{C}} M_{\mathrm{U}}(t) \\ S_{\mathrm{T}}(t) &= k_{\mathrm{C}} M_{\mathrm{T}}(t) \end{aligned}\right\} \quad t \geqslant T \tag{A1.4}$$

and are zero for earlier times.

In the present case study (probabilistic case) T, k_{I} and k_{C} all vary independently.

A1.2 Geosphere layers

The geosphere has two layers, each of which is one-dimensional with path length $l^{(k)}$, where k is 1 or 2 indicating the layer. The sub-model includes advection, equilibrium sorption, and longitudinal dispersion. The governing equations are

$$\begin{aligned} R_{\mathrm{I}}^{(k)} \frac{\partial C_{\mathrm{I}}^{(k)}}{\partial t} + v^{(k)} \frac{\partial C_{\mathrm{I}}^{(k)}}{\partial x} - d^{(k)} v^{(k)} \frac{\partial^2 C_{\mathrm{I}}^{(k)}}{\partial x^2} &= -\lambda_{\mathrm{I}} R_{\mathrm{I}}^{(k)} C_{\mathrm{I}}^{(k)} \\ R_{\mathrm{N}}^{(k)} \frac{\partial C_{\mathrm{N}}^{(k)}}{\partial t} + v^{(k)} \frac{\partial C_{\mathrm{N}}^{(k)}}{\partial x} - d^{(k)} v^{(k)} \frac{\partial^2 C_{\mathrm{N}}^{(k)}}{\partial x^2} &= -\lambda_{\mathrm{N}} R_{\mathrm{N}}^{(k)} C_{\mathrm{N}}^{(k)} \\ R_{\mathrm{U}}^{(k)} \frac{\partial C_{\mathrm{U}}^{(k)}}{\partial t} + v^{(k)} \frac{\partial C_{\mathrm{U}}^{(k)}}{\partial x} - d^{(k)} v^{(k)} \frac{\partial^2 C_{\mathrm{U}}^{(k)}}{\partial x^2} &= -\lambda_{\mathrm{U}} R_{\mathrm{U}}^{(k)} C_{\mathrm{U}}^{(k)} + \lambda_{\mathrm{N}} R_{\mathrm{N}}^{(k)} C_{\mathrm{N}}^{(k)} \\ R_{\mathrm{T}}^{(k)} \frac{\partial C_{\mathrm{T}}^{(k)}}{\partial t} + v^{(k)} \frac{\partial C_{\mathrm{T}}^{(k)}}{\partial x} - d^{(k)} v^{(k)} \frac{\partial^2 C_{\mathrm{T}}^{(k)}}{\partial x^2} &= -\lambda_{\mathrm{T}} R_{\mathrm{T}}^{(k)} C_{\mathrm{T}}^{(k)} + \lambda_{\mathrm{U}} R_{\mathrm{U}}^{(k)} C_{\mathrm{U}}^{(k)} \end{aligned} \tag{A1.5}$$

The retardation coefficients for the chain are related by

$$\begin{aligned} R_{\mathrm{N}}^{(k)} &= R_{0\mathrm{N}}^{(k)} \gamma_{\mathrm{C}}^{(k)} \\ R_{\mathrm{U}}^{(k)} &= R_{0\mathrm{U}}^{(k)} \gamma_{\mathrm{C}}^{(k)} \\ R_{\mathrm{T}}^{(k)} &= R_{0\mathrm{T}}^{(k)} \gamma_{\mathrm{C}}^{(k)} \end{aligned} \tag{A1.6}$$

where $\gamma_{\mathrm{C}}^{(k)}$ varies and $R_{0\mathrm{N}}^{(k)}$, $R_{0\mathrm{U}}^{(k)}$ and $R_{0\mathrm{T}}^{(k)}$ are fixed. For each layer $v^{(k)}$ and $l^{(k)}$ vary.

For our purposes it is simpler to work with equations for the fluxes, $F_i^{(k)}(x, t)$:

$$\begin{aligned}
R_{\mathrm{I}}^{(k)}\frac{\partial F_{\mathrm{I}}^{(k)}}{\partial t} + v^{(k)}\frac{\partial F_{\mathrm{I}}^{(k)}}{\partial x} - d^{(k)}v^{(k)}\frac{\partial^2 F_{\mathrm{I}}^{(k)}}{\partial x^2} &= -\lambda_{\mathrm{I}}R_{\mathrm{I}}^{(k)}F_{\mathrm{I}}^{(k)} \\
R_{\mathrm{N}}^{(k)}\frac{\partial F_{\mathrm{N}}^{(k)}}{\partial t} + v^{(k)}\frac{\partial F_{\mathrm{N}}^{(k)}}{\partial x} - d^{(k)}v^{(k)}\frac{\partial^2 F_{\mathrm{N}}^{(k)}}{\partial x^2} &= -\lambda_{\mathrm{N}}R_{\mathrm{N}}^{(k)}F_{\mathrm{N}}^{(k)} \\
R_{\mathrm{U}}^{(k)}\frac{\partial F_{\mathrm{U}}^{(k)}}{\partial t} + v^{(k)}\frac{\partial F_{\mathrm{U}}^{(k)}}{\partial x} - d^{(k)}v^{(k)}\frac{\partial^2 F_{\mathrm{U}}^{(k)}}{\partial x^2} &= -\lambda_{\mathrm{U}}R_{\mathrm{U}}^{(k)}F_{\mathrm{U}}^{(k)} + \lambda_{\mathrm{N}}R_{\mathrm{N}}^{(k)}F_{\mathrm{N}}^{(k)} \\
R_{\mathrm{T}}^{(k)}\frac{\partial F_{\mathrm{T}}^{(k)}}{\partial t} + v^{(k)}\frac{\partial F_{\mathrm{T}}^{(k)}}{\partial x} - d^{(k)}v^{(k)}\frac{\partial^2 F_{\mathrm{T}}^{(k)}}{\partial x^2} &= -\lambda_{\mathrm{T}}R_{\mathrm{T}}^{(k)}F_{\mathrm{T}}^{(k)} + \lambda_{\mathrm{U}}R_{\mathrm{U}}^{(k)}F_{\mathrm{U}}^{(k)}
\end{aligned} \tag{A1.7}$$

The initial conditions are zero concentration (and flux) for all x in both layers.

The boundary conditions for each geosphere layer are specified as follows. At the beginning of the layer, the flux is equal to that output by the source or previous layer. The solution in the layer is then also required to be that which would be obtained in a semi-infinite layer under the condition that flux → zero at $x \to \infty$. (This use of conditions at infinity is a requirement to make the integrals in the exact solution tractable.)

Thus, for the first layer we have

$$\left.\begin{aligned} F_i^{(1)}(0, t) &= S_i(t) \\ F_i^{(1)}(\infty, t) &\to 0 \end{aligned}\right\} \quad i = \mathrm{I, N, U, T}, \tag{A1.8}$$

and the flux at the end of the layer is

$$G_i^{(1)}(t) = F_i^{(1)}(l^{(1)}, t) \quad i = \mathrm{I, N, U, T}. \tag{A1.9}$$

For the second layer we have

$$\left.\begin{aligned} F_i^{(2)}(0, t) &= G_i^{(1)}(t) \\ F_i^{(2)}(\infty, t) &\to 0 \end{aligned}\right\} \quad i = \mathrm{I, N, U, T}, \tag{A1.10}$$

and the flux at the end of the layer (the output to the biosphere) is

$$G_i^{(2)}(t) = F_i^{(2)}(l^{(2)}, t) \quad i = \mathrm{I, N, U, T}. \tag{A1.11}$$

A1.3 Biosphere

The biosphere sub-model is very simple. The full geosphere flux is assumed to enter a stream, which is used for drinking water. The dose received depends on the ratio of the drinking water consumption and the stream flow rate. The dose arising from nuclide i is calculated as

$$D_i(t) = \beta_i \frac{w}{W} G_i^{(2)}(t) \quad i = \text{I, N, U, T.} \tag{A1.12}$$

where β_i is a dose conversion factor. The stream flow rate W is taken as variable, while w and β_i are fixed.

Appendix 2: Questionnaire and Reference Results

General Notes

1. Participants are encouraged to make their contribution complete by giving all requested information.
2. Please use separate copies of this questionnaire if you wish to submit more than one set of results (e.g. using different sampling methods).
3. Result values should be provided to 4 significant figures.
4. Specified times are from the time of the start of the study, i.e. vault closure.
5. In the questions, 'dose' means annual effective dose equivalent.
6. Radionuclide dose values of less than 10^{-15} Sv/yr may be considered zero.

Section A: General Information about PSA Code

A1. Name and address of contact person

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.....

.....

A2. Name of Code.....

A3. Version Number and Date .....

A4. Submodel solution technique (numerical/analytical/other)

Source.....

Geosphere .....

Biosphere.....

A5. Sampling technique .....

Any special features.....

.....

A6. Number of runs in case .....

A7. Number of time steps per run (if applicable) .....

Section B: Deterministic Results

B1. Radionuclide flux (mols/yr) at given time (yrs) from Source, $S_i(t)$ (equation A1.4)

Nuclide	Fixed Case 1		Fixed Case 2		Fixed Case 3	
	Flux	Time	Flux	Time	Flux	Time
I–129		1×10^3		1×10^3		1×10^3
Exact result:	1.234E–4		3.674E–2		1.000E–1	
Np–237		1×10^5		1×10^5		1×10^5
Exact result:	3.565E–3		2.154E–3		8.769E–4	
U–233		1×10^5		1×10^5		1×10^5
Exact result:	3.329E–4		2.011E–4		8.187E–5	
Th–229		1×10^5		1×10^5		1×10^5
Exact result:	1.585E–5		9.576E–6		3.899E–6	

B2. Peak radionuclide flux (mols/yr) and Time of peak (yrs) from Geosphere Layer 1, $\max_t G_i^{(1)}(t)$ (equation A1.9)

Nuclide	Fixed Case 1		Fixed Case 2		Fixed Case 3	
	Peak flux	Time of peak	Peak flux	Time of peak	Peak flux	Time of peak
I–129 Exact result:	1.061E–1	9.55E2	1.169E–2	1.10E4	4.140E–3	4.91E4
Np–237 Exact result:	2.518E–3	3.07E5	3.217E–4	1.92E6	2.526E–6	1.17E7
U–233 Exact result:	6.952E–4	5.24E4	1.477E–4	1.12E6	3.139E–6	9.17E6
Th–229 Exact result:	3.122E–6	6.63E4	6.860E–7	1.12E6	1.458E–8	9.17E6

B3. Peak dose (Sv/yr) and Time of peak (yrs), $\max_t D_i(t)$ (equation A1.12)

Nuclide	Fixed Case 1		Fixed Case 2		Fixed Case 3	
	Peak dose	Time of peak	Peak dose	Time of peak	Peak dose	Time of peak
I–129 Exact result:	1.218E–5	1.47E3	3.485E–7	2.10E4	3.323E–8	1.08E5
Np–237 Exact result:	3.535E–5	4.62E5	3.219E–7	4.86E6	2.592E–11	2.45E7
U–233 Exact result:	9.209E–6	6.95E4	2.072E–7	3.43E6	3.596E–11	2.12E7
Th–229 Exact result:	1.265E–5	8.33E4	2.937E–7	3.43E6	5.095E–11	2.12E7

Section C: Stochastic Results

C1. Statistics of Dose (Sv/yr) from I–129 at given times (yrs), i.e. of $D_I(t)$.

Mean and Standard Deviation (equations 3.1 to 3.4)

Time	1×10^4	2×10^4	5×10^4	1×10^5	2×10^5	5×10^5
Mean of dose at time, $\hat{E}(D_I(t))$						
Exact result:	3.779E–8	7.854E–8	5.382E–8	2.353E–8	9.981E–9	2.822E–9
Std. deviation of dose at time, $\hat{\sigma}(D_I(t))$						

Confidence limits on estimate of mean, $\hat{E}(D_I(t))$ based on Chebyshev's Inequality (equation 3.6)

Time	1×10^4	2×10^4	5×10^4	1×10^5	2×10^5	5×10^5
Lower 95% confidence limit						
Upper 95% confidence limit						

Confidence limits on estimate of mean, $\hat{E}(D_I(t))$, based on tested normality of mean (equations 3.7, 3.8)

Time	1×10^4	2×10^4	5×10^4	1×10^5	2×10^5	5×10^5
Number of batches, *M*						
Shapiro–Wilk *W*–statistic						
Lower 95% confidence limit						
Upper 95% confidence limit						

Confidence limits on estimate of mean, $\hat{E}(D_I(t))$, based on another method *(optional)*

Time	1×10^4	2×10^4	5×10^4	1×10^5	2×10^5	5×10^5
Lower 95% confidence limit						
Upper 95% confidence limit						
Method used, and any relevant data (give details of method on a separate sheet)						

C2. Mean and standard deviation of Maximum dose (Sv/yr) from I–129 up to given times (yrs), i.e. of $P_I(t)$.

Time	1×10^4	2×10^4	5×10^4	1×10^5	2×10^5	5×10^5
Mean of maximum dose up to time, $\hat{E}(P_I(t))$						
Std. deviation of maximum dose up to time, $\hat{\sigma}(P_I(t))$						

C3. Statistics of total dose (Sv/yr) from Chain (Np–237, U–233, Th–229) at given times (yrs), i.e. of $D_C(t)$.

Mean and Standard Deviation (equations 3.1 to 3.4)

Time	5×10^5	1×10^6	2×10^6	5×10^6	1×10^7
Mean of dose at time, $\hat{E}(D_C(t))$ Exact result:	2.762E–8	4.905E–8	6.506E–8	6.475E–8	1.845E–8
Std. deviation of dose at time, $\hat{\sigma}(D_C(t))$					

Confidence limits on estimate of mean, $\hat{E}(D_C(t))$, based on Chebyshev's Inequality (equation 3.6)

Time	5×10^5	1×10^6	2×10^6	5×10^6	1×10^7
Lower 95% confidence limit					
Upper 95% confidence limit					

Confidence limits on estimate of mean, $\hat{E}(D_C(t))$, based on tested normality of mean (equations 3.7, 3.8)

Time	5×10^5	1×10^6	2×10^6	5×10^6	1×10^7
Number of batches, *M*					
Shapiro–Wilk *W*–statistic					
Lower 95% confidence limit					
Upper 95% confidence limit					

Confidence limits on estimate of mean, $\hat{E}(D_C(t))$ based on another method *(optional)*

Time	5×10^5	1×10^6	2×10^6	5×10^6	1×10^7
Lower 95% confidence limit					
Upper 95% confidence limit					
Method used, and any relevant data (give details of method on a separate sheet)					

C4. Mean and standard deviation of Maximum dose (Sv/yr) from Chain (Np–237, U–233, Th–229) at given times (yrs), i.e. of $P_C(t)$.

Time	5×10^5	1×10^6	2×10^6	5×10^6	1×10^7
Mean of maximum dose up to time, $\hat{E}(P_C(t))$					
Std. deviation of maximum dose up to time, $\hat{\sigma}(P_C(t))$					

C5. Distribution of dose (Sv/yr) from I–129 at given times, $D_I(t)$.
Give frequencies of dose values in each specified range.

Dose range	Time					
	1×10^4	2×10^4	5×10^4	1×10^5	2×10^5	5×10^5
≥ 0 , $<10^{-15}$						
$\geq 10^{-15}$, $<10^{-14.5}$						
$\geq 10^{-14.5}$, $<10^{-14}$						
$\geq 10^{-14}$, $<10^{-13.5}$						
$\geq 10^{-13.5}$, $<10^{-13}$						
$\geq 10^{-13}$, $<10^{-12.5}$						
$\geq 10^{-12.5}$, $<10^{-12}$						
$\geq 10^{-12}$, $<10^{-11.5}$						
$\geq 10^{-11.5}$, $<10^{-11}$						
$\geq 10^{-11}$, $<10^{-10.5}$						
$\geq 10^{-10.5}$, $<10^{-10}$						
$\geq 10^{-10}$, $<10^{-9.5}$						
$\geq 10^{-9.5}$, $<10^{-9}$						
$\geq 10^{-9}$, $<10^{-8.5}$						
$\geq 10^{-8.5}$, $<10^{-8}$						
$\geq 10^{-8}$, $<10^{-7.5}$						
$\geq 10^{-7.5}$, $<10^{-7}$						
$\geq 10^{-7}$, $<10^{-6.5}$						
$\geq 10^{-6.5}$, $<10^{-6}$						
$\geq 10^{-6}$, $<10^{-5.5}$						
$\geq 10^{-5.5}$, $<10^{-5}$						
$\geq 10^{-5}$, $<10^{-4.5}$						
$\geq 10^{-4.5}$, $<10^{-4}$						
$\geq 10^{-4}$, $<10^{-3.5}$						
$\geq 10^{-3.5}$, $<10^{-3}$						
$\geq 10^{-3}$						

C6. Distribution of dose (Sv/yr) from Chain (Np–237, U–233, Th–229) at given times, $D_C(t)$. Give frequencies of dose values in each specified range.

Dose range	Time				
	5×10^5	1×10^6	2×10^6	5×10^6	1×10^7
≥ 0 , $<10^{-15}$					
$\geq 10^{-15}$, $<10^{-14.5}$					
$\geq 10^{-14.5}$, $<10^{-14}$					
$\geq 10^{-14}$, $<10^{-13.5}$					
$\geq 10^{-13.5}$, $<10^{-13}$					
$\geq 10^{-13}$, $<10^{-12.5}$					
$\geq 10^{-12.5}$, $<10^{-12}$					
$\geq 10^{-12}$, $<10^{-11.5}$					
$\geq 10^{-11.5}$, $<10^{-11}$					
$\geq 10^{-11}$, $<10^{-10.5}$					
$\geq 10^{-10.5}$, $<10^{-10}$					
$\geq 10^{-10}$, $<10^{-9.5}$					
$\geq 10^{-9.5}$, $<10^{-9}$					
$\geq 10^{-9}$, $<10^{-8.5}$					
$\geq 10^{-8.5}$, $<10^{-8}$					
$\geq 10^{-8}$, $<10^{-7.5}$					
$\geq 10^{-7.5}$, $<10^{-7}$					
$\geq 10^{-7}$, $<10^{-6.5}$					
$\geq 10^{-6.5}$, $<10^{-6}$					
$\geq 10^{-6}$, $<10^{-5.5}$					
$\geq 10^{-5.5}$, $<10^{-5}$					
$\geq 10^{-5}$, $<10^{-4.5}$					
$\geq 10^{-4.5}$, $<10^{-4}$					
$\geq 10^{-4}$, $<10^{-3.5}$					
$\geq 10^{-3.5}$, $<10^{-3}$					
$\geq 10^{-3}$					

C7. Mean dose (Sv/yr) against sample size for I–129 at 2×10^4 years (definitions as in question C1.) Supply means and confidence intervals for whatever range of sample sizes is convenient. Add futher columns, or use fewer, as necessary.

Are the different samples independent, or does each batch include the smaller ones?

.....

Sample size					
Estimate, from sample, of mean dose at time, $\hat{E}(D_I(t))$					
Lower and upper 95% confidence limits (Chebyshev)					
Lower and upper 95% confidence limits (tested normality)					
Normality test details (M, W)					
Lower and upper 95% confidence limits (other method)					
Relevant data for other method					

C8. Mean dose (Sv/yr) against sample size for Chain (Np–237, U–233, Th–229) at 2×10^6 years (definitions as in question C3.)
Supply means and confidence intervals for whatever range of sample sizes is convenient. Add futher columns, or use fewer, as necessary.

Are the different samples independent, or does each batch include the smaller ones?

.....

Sample size					
Estimate from sample of mean dose at time, $\hat{E}(D_C(t))$					
Lower and upper 95% confidence limits (Chebyshev)					
Lower and upper 95% confidence limits (tested normality)					
Normality test details (M, W)					
Lower and upper 95% confidence limits (other method)					
Relevant data for other method					

C9. Rank nuclides by contribution to mean dose at specified times (years).

Time	Ranked contributors (radionuclides) greatest . . . . . least
10^4	
2×10^4	
5×10^4	
10^5	
2×10^5	
5×10^5	
10^6	
2×10^6	
5×10^6	
10^7	

ANNEX B

Brief Code Descriptions

CODE: LISA.SCK, Version 4.0-E

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For the Level E exercise, the LISA.SCK code treated the different parts of the repository system as follows. The source model consisted of two subroutines: the first one solved analytically the Bateman equations and the second one calculated analytically the dissolution rate of the waste form and radionuclide releases from the vault. In the geosphere model, the NUCDIS2 code solved numerically the advection-dispersion equation using the Crank-Nicolson technique; the theoretical boundary condition, zero concentration at infinity, is approximated by the boundary condition, zero concentration at $x = 2L$, where L is the thickness of the geosphere layer under consideration. The biosphere submodel was reduced to a simple flux-to-dose conversion factor.

Identical time steps were used for both geosphere layers; the time steps were increased exponentionally to a maximum value that depended on the shortest half-life in the decay series. The source subroutines calculated the radionuclide release rates at each (geosphere) time step. A log-log interpolation routine was used to provide results at the reference times.

The parameter sampling method used was Latin Hypercube Sampling. The relatively small number of runs in the simulation did not allow any meaningful combination of the runs into batches.

CODE: SYVAC3-LE01

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SYVAC3 treats each time-dependent variable as a time series with uneven time-steps; time-steps are small when the variable is changing nonlinearly, and large when the variable varies linearly with time. The chief source of error in SYVAC3 calculations is the fitting error involved in representing smooth functions of time as piecewise linear functions. In constructing such a time series, new times are introduced until the estimated error in the integral of the entire time series falls below a specified fractional error. For the Level E exercise, time series were allowed to have from 20 to 250 time steps. The specified fractional error was 0.1% for deterministic runs and 2% for stochastic runs.

SYVAC3 has a general compartment solver to calculate a time series for the amount of material that accumulates (or is left) in a compartment. The compartment solver handles a time-varying input flow, a capacity-limited output flow, formation from a parent within the compartment (i.e., radioactive decay), and linear loss within the compartment (i.e., due to decay). It uses a response function/convolution technique to calculate the accumulated amount in the compartment. For the Level E exercise, release from the waste form was treated as a linear loss rate. The compartment model solved for the remaining inventory and for the release rate, both as functions of time. A special version of the compartment model was developed to deal with a time-varying response funtion (i.e., the rate of loss during the first 100 years differed from the rate later on). It will now become a standard SYVAC3 component.

The transport equations and boundary conditions in each layer of the geosphere were solved exactly using a response function technique [W.F. Heinrich and T. Andres, Response Functions of the Convection-Dispersion Equations Describing Radionuclide Migration in a Semi-Infinite Medium; Ann. Nucl. Energy, 12(12), 1985, pp. 685-691]. That is, the release-rate time series from the vault were convoluted with geosphere response functions for the first layer. The time series for release from the first layer were convoluted with geosphere response functions for the second layer to yield the release time series for that layer.

The biosphere was solved by evaluating a scalar "nuclide dose conversion ratio" and multiplying the time series for release from the second geosphere layer by this scalar to yield a dose time series.

Simple Random Sampling was used for stochastic simulations. Parameters for all distributions were generated by using the inverse cumulative distribution transform on uniformly distributed variates between 0 and 1. Sampling in SYVAC3 is performed for each simulation just before that simulation is carried out. Deterministic simulations were carried out by changing the sampling method to read values directly from a computer file.

Mean values, standard deviations, and confidence limits were calculated as in the report.

CODE: COSMOS-S/D, Version 2

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The COSMOS-S/D code system consists of a central routine, known as COSMOS, that models radionuclide migration along pathways that may contain parallel branches. Preprocessor and postprocessor routines surround the central routine. One of the preprocessors generates sample parameter sets using simple Monte Carlo sampling. Once COSMOS has computed doses using these sample sets, a postprocessor routine analyses these sample realisations using the same statistical formulae given in the report. If batches of sample realisations are wanted, and if ten batches out of N samples are wanted, then the first batch consists of the first N/10 sample realisations, and so on.

COSMOS consists of submodels of each of the physical processes involved in radionuclide migration. Each submodel calculates values for one or more single-subscript arrays that represent radionuclide concentrations as functions of time. The time grid consists of a fixed number of points separated by intervals of constant width, and applies throughout the submodel. The mathematical equations describing the physical systems are solved analytically as far as possible, but the forcing functions of these equations are represented by the concentration arrays. To incorporate these in the solution, a numerical integration over time is required, usually using a simple trapezoidal method. In the last submodel, concentrations are changed to doses by computing pathway dose-conversion factors, which involve algebraic expressions. No decay chains are considered.

For the Level E exercise, submodels representing physical processes not required by the specification were deactivated. The submodels representing the vault were replaced by a submodel consisting of algebraic expressions representing the analytical solution of the vault equations given in the specification. The subroutine that computes pathway dose-conversion factors was replaced by data provided in the specification.

Aside from decay-chain terms, the system of equations describing the Level E geosphere is analogous to those used in COSMOS. The relevant submodel, therefore, was left unmodified so that the Level E exercise could assist with verification of the COSMOS geosphere submodel.

Because of the decay-chain limitation in COSMOS, only results for I-129 were submitted. Moreover, because of the time-step limitation in COSMOS, two sets of stochastic results were submitted. One employed a time step of 1000 years, spanning the entire time of simulation, and the other had a time step of 100 years, spanning the first tenth of the simulation period. More detailed results are thus available for the period where rapid changes and peaks in dose occur. It is intended, then, that the two runs be treated as one with the results for the finer time grid applying in the regions where simulation times overlap.

CODE: JAERI (tentative), Version 1.2

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JAERI, Tokai Research Establishment
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Ibaraki-ken
Japan

The code JAERI (tentative), Version 1.2 is composed of vault, geosphere, and biosphere submodels. The vault submodel represents release of radionuclides from the repository. The fluxes from the repository were calculated analytically in the Level E exercise, and these fluxes were used as a source term for the geosphere. The geosphere submodel used in the Level E exercise is an extended version of MGRAT03. Because MGRAT03 can calculate the one-dimensional migration of radionuclide chains only for a one-layer geologic medium, it was extended in order to handle multilayer cases based on work by J. Hadermann and J. Patry. This submodel is solved analytically by the Laplace transform method, and the integration is done by the Gaussian-Legendre method. This submodel includes advection, equilibrium sorption, and longitudinal dispersion. The biosphere submodel is based on the CIRCLE code, a tool for analysing the dynamics of linear compartment models linked with the parameter sampling code, LHS (Latin Hypercube Sampling), as well as with a code for sensitivity analyses. A simple multiplicative factor was used to calculate dose in the biosphere model used for the Level E exercise, however. This factor contains stream dilution and human consumption.

The JAERI code incorporates two parameter sampling methods: Latin Hypercube Sampling and Random Sampling. The former was used for the Level E exercise.

CODE: PROPER Monitor, Version 0.0

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Source, geosphere, and biosphere submodels were specially developed for the Level E exercise for use with the PROPER monitor.

The source submodel used analytical solutions of the differential equations and the PROPER time-series manager to provide the result at certain time points (an adaptive algorithm).

The geosphere submodel used analytical response-function solutions of the differential equations for I-129 and Np-237 and Laplace-space analytical response functions for U-233 and Th-229. Laplace inversion was accomplished by the PROPER numerical Laplace-inversion routine, which is based on Talbot's (1979) method. Response time series were managed by the PROPER time-series manager, and, convolution integration, using a routine in PROPER, provided the output time series. The same submodel was used for both geosphere layers (i.e., twice).

The biosphere submodel simply multiplied the time series from geosphere layer 2 by the appropriate factors to give the output-dose time series.

The parameter sampling method used was crude Monte Carlo. The full 1000-realisation sample was divided into 25 batches with 40 realisations in each. This subdivision is necessary when PROPER's confidence-band measurement option is used. The method is different from that prescribed in the Level E specification. In this case, the 0.95 fractiles on the cumulative curves for the doses at 2×10^4 and 2×10^6 a for I-129 and the Neptunium chain, respectively, were followed through the simulation. The precision was expressed as the relative uncertainty in the value of that fractile at the 0.90 confidence level. This confidence interval is obtained using Chebyshev's Inequality, based on the second moment about the mean of the fractile for each batch. The reason why fractiles are used instead of the mean of the distribution is the notion that the moments of a distribution are poor substitutes for the distribution itself. Chebyshev confidence intervals on the means of the distributions were nonetheless also computed in order to complete the Level E questionnaire.

CODE: SYVAC/SU, Version 2

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The source submodel was specially written for the Level E exercise. The differential equations were solved analytically and calculated at specified time points by the source code.

The standard SYVAC/SU geosphere submodel was used. The geosphere is treated as a semi-infinite homogeneous medium. The differential equation for a single nuclide and the coupled partial differential equations for members of a decay chain, solved in Laplace space and with their solution inverted, are solved analytically as a response function for unit releases. This response function is then convoluted with the source term or the release from the first geopshere layer. The convolution integral is solved using Simpson's Rule. The nuclide concentration at a certain time, as used in the Simpson integration, is calculated by the source code or by linear interpolation from the release of the first geosphere layer.

The biosphere submodel was specially written for the Level E exercise. The final release to the biosphere was calculated at fixed logarithmic, equidistant time points.

The parameter sampling method used was crude Monte Carlo. Mean values, standard deviations, and confidence intervals were calculated as in the report.

CODE: MASCOT, Version PRAM2D

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Both the output fluxes from the source model and the response functions for each geosphere layer can readily be written out analytically as Laplace transforms for the Level E exercise. For each set of sampled parameters, MASCOT evaluates these Laplace functions at points along a complex contour. The Laplace functions for the submodels are multiplied with each other - equivalent to convoluting the time-domain responses. The resultant function values on the contour are combined by Talbot's (1979) method to invert the Laplace transform. The program adaptively adjusts the contour shape to obtain good accuracy.

The parameter sampling method used was simple Monte Carlo. The estimators used for means, standard deviations, and confidence limits were as given in the report.

CODE: SYVAC-D, Version 1.0

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The SYVAC-D code is composed of three physical submodels, namely the near-field, geosphere, and biosphere models. The near-field submodel simulates release of radionuclides through the different engineered barriers. It is numerical with a variable time step. The one-dimensional geosphere submodel is solved analytically. Each geosphere pathway is solved independently in response to a unit Dirac, and a zero concentration at infinite distance is assumed. Finally, the biosphere submodel is reduced to a dose-rate/flux multiplier.

The structure of the near-field model does not allow this part of SYVAC-D to be reduced to a simple release rate. It has therefore been replaced by a subroutine which solves numerically the model used in the Level E exercise. However, variable time stepping was retained in order to preserve the entire executive of SYVAC-D for the exercise. An interpolation routine allows for the near-field time steps to coincide with the user-defined time steps employed in the geosphere model. The different sections are then convoluted and the biosphere multiplier is applied to the results.

The stochastic analysis is obtained by Monte Carlo sampling within the code. When convergence is not obtained, Importance Sampling is used. The basis of this variance-reduction method is to resample iteratively certain random variables according to the sensitivity of the results. For Importance Sampling, samples are taken from a multivariate density distribution, S(x), and mean dose is estimated from

$$D_t = \frac{1}{N} \sum_i H_t(x_i)\, P(x_i) \,/\, S(x_i)$$

where D_t is mean dose at time t, H_t is the dose at time t resulting from the parameter vector $\underline{x} = (x_1, x_2, \ldots, x_k)$, P(x) is the subjective distribution function of

$$P(\underline{x}) = \prod_j P(x_j),$$

and $S(x_j)$ is an estimate of the marginal distribution of $H(x_j)\, P(x_j)$.

All statistics required in the questionnaire for Importance Sampling results (i.e., standard deviation, Shapiro-Wilk statistic, and distribution of dose histograms) are of the quantity $(H_i P_i)/S_i$, where H_i is the dose for run i, P_i is the subjective probability density of run i, and S_i is the sampling probability density of run i.

CODE: ESP/T

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The ESP/T code contains three submodels to represent the near field, the far field (geosphere), and the biosphere. The near-field model represents release of radionuclides from the repository; for the Level E exercise, this was done by calculating analytically a flux-versus-time history, which was used as a source term for the geosphere. The geosphere is represented by a one-dimensional finite-difference model, TROUGH-1D, which numerically solves the differential equations for radionuclide transport, using the source term calculated by the near-field model, and assuming zero concentration of all species at infinite distance. Time and space step sizes are calculated to suit the parameter values; this is necessary as the results obtained are dependent on the time and space steps used. The biosphere model used for the Level E exercise was a simple multiplicative factor to convert the flux into the biosphere to a dose, simulating stream dilution and human consumption.

A log-log interpolation routine is used to take the results for each run, for time steps specific to that run, and to provide results at a set of reference times.

A Latin Hypercube Sampling (LHS) routine was used to sample parameter values from the ranges specified. In selecting N sets of parameters, the LHS routine divides the range of each parameter into N nonoverlapping intervals of equal probability. One value is then selected at random from the probability distribution in each of these intervals. The N values of the first parameter are then paired randomly with the N values of the second parameter. These N pairs are then paired randomly with the N values of the third parameter, and so on. Thus, N sets of parameter values are constructed and, hence, N runs of the models are performed. In this study, it was assumed that none of the parameters were correlated. As mentioned above, some of the sampled parameters are used in determining suitable time steps for the run to which they apply; time steps were calculated based on an estimate of the time at which the peak dose would arise.

All dose values are given equal weight in calculating statistical results, as it is assumed that the sampling procedure assigns weights implicitly when selecting sets of parameter values. Where the statistical calculations require the division of dose results into batches, e.g., the Shapiro-Wilk statistic, this division is not random; for a batch size h, the first b runs are batch 1, the next b are batch 2, etc. Because the sampling is not necessarily completely random, neither is the batch selection.

CODE: LISA, Version 4.0

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Either Latin Hypercube Sampling or Simple Random Sampling can be used with the LISA code; the latter parameter sampling scheme was used for the Level E exercise. Input variables can be correlated with LISA; spurious correlations were eliminated in the Level E exercise by imposing low correlations (< 0.1) between the input variables. LISA incorporates source, geosphere, and biosphere submodels. The biosphere submodel, although still available in the code module library, is no longer used; lumped biosphere transfer coefficients are used instead. In LISA the submodels communicate with each other through time series (of, e.g., fluxes in mol/a or Bq/a) whose time step changes from one code module to the next. Interpolation subroutines are employed.

Several modifications to LISA were made for the Level E exercise. The source submodel was bypassed. An exponential waste degredation-leach rate function was instead inserted in the submodel containing the Bateman equations. The TROUGH code was used for the geopshere after solving a number of time-stepping problems created by existing versions of the code. Treatment of the biosphere was straightforward.

Different time steps were used for the deterministic and the stochastic simulations in order to save computor time. The estimators used for means, standard deviations, and confidence limits were as given in the report. Statistical computations were performed using the SPOP postprocessor. Computing times used for the entire exercise (about 2000 runs of LISA, plus several executions of SPOP) were on the order of 50 cpu hours on the Ispra Amdhal V8 computer.

ANNEX C

Tables of Original Results from Case Studies

This Annex contains selected Tables of original results from the case studies, corresponding to nearly all of those results presented and discussed in Sections 2 and 3 of this report, plus some additional results. These results were submitted using the questionnaire included in Annex A of the report. Results tabulated here are drawn from Sections B ("Deterministic Results") and C ("Stochastic Results) of the questionnaire, and are numbered in accordance with the corresponding part of the questionnaire.

The data in this Annex are provided in order that interested readers of this report may be in a position to disentangle clusters of data illustrated in Sections 2 and 3 of the report, should they so wish. In addition, the data are provided so that readers may perform at least some additional statistical analyses of the contributed data, should they so wish.

All of the final results submitted by participants, including the results provided here and those not provided here, are freely available in both paper and machine-readable form from the NEA Data Bank to interested readers of this report. These data are numerous and are not all given here in order to maintain this Annex at a reasonable length.

Table B1.1 I^{129} Radionuclide Flux (mols/yr) at 10^3 years

Participant	Case 1	Case 2	Case 3
A EXACT	1.2340E-04	3.6740E-02	0.1000
B LISA.SCK-4.0	1.2340E-04	3.6740E-02	0.1000
C SYVACD1000			
D SYVACD10000	1.2340E-04	3.6900E-02	0.1000
E MASCOT1000	1.2340E-04	3.6730E-02	0.1000
F MASCOT4000	1.2340E-04	3.6730E-02	0.1000
G JAERI-LHS1.1	1.2340E-04	3.6740E-02	0.1000
H COSMOS1	1.2340E-04	3.6740E-02	0.1000
I SYVAC/SU	1.2340E-04	3.6740E-02	0.1000
J PROPER	1.3200E-04	3.6780E-02	0.1000
K ESP			
L LISA4-JRC	1.2340E-04	3.6740E-02	0.0987
N SYVAC3-LE1	1.5670E-04	3.6820E-02	0.0002

Table B1.2 Np^{337} Radionuclide Flux (mols/yr) at 10^5 years

Participant	Case 1	Case 2	Case 3
A EXACT	3.5650E-03	2.1540E-03	8.7690E-04
B LISA.SCK-4.0	3.5650E-03	2.1540E-03	8.7690E-04
C SYVACD1000	3.5600E-03	2.1000E-03	8.7600E-04
D SYVACD10000	3.5600E-03	2.1000E-03	8.7600E-04
E MASCOT1000	3.5650E-03	2.1540E-03	8.7690E-04
F MASCOT4000	3.5650E-03	2.1540E-03	8.7690E-04
G JAERI-LHS1.1	3.5650E-03	2.1540E-03	8.7690E-04
H COSMOS1			
I SYVAC/SU	3.5650E-03	2.1540E-03	8.7690E-04
J PROPER	3.5650E-03	2.1550E-03	8.7690E-04
K ESP			
L LISA4-JRC	3.5650E-03	2.1540E-03	8.7690E-04
N SYVAC3-LE1	3.5710E-03	2.1540E-03	8.7730E-04

Table B1.3 U^{233} **Radionuclide Flux (mols/yr) at** 10^5 **years**

Participant	Case 1	Case 2	Case 3
A EXACT	3.3290E-04	2.0110E-04	8.1870E-05
B LISA.SCK-4.0	3.3290E-04	2.0110E-04	8.1870E-05
C SYVACD1000	3.3300E-04	2.0400E-04	8.1700E-05
D SYVACD10000	3.3300E-04	2.0400E-04	8.1700E-05
E MASCOT1000	3.3290E-04	2.0110E-04	8.1870E-05
F MASCOT4000	3.3290E-04	2.0110E-04	8.1870E-05
G JAERI-LHS1.1	3.3290E-04	2.0110E-04	8.1870E-05
H COSMOS1			
I SYVAC/SU	3.3290E-04	2.0110E-04	8.1870E-05
J PROPER	3.3290E-04	2.0110E-04	8.1900E-05
K ESP			
L LISA4-JRC	3.3290E-04	2.0110E-04	8.1880E-05
N SYVAC3-LE1	3.3350E-04	2.0120E-04	8.1910E-05

Table B1.4 Th^{229} **Radionuclide Flux (mols/yr) at** 10^5 **years**

Participant	Case 1	Case 2	Case 3
A EXACT	1.5850E-05	9.5760E-06	3.8990E-06
B LISA.SCK-4.0	1.5850E-05	9.5760E-06	3.8990E-06
C SYVACD1000	1.5800E-05	9.6800E-06	3.8800E-06
D SYVACD10000	1.5800E-05	9.6800E-06	3.8800E-06
E MASCOT1000	1.5850E-05	9.5760E-06	3.8990E-06
F MASCOT4000	1.5850E-05	9.5760E-06	3.8990E-06
G JAERI-LHS1.1	1.5850E-05	9.5760E-06	3.8990E-06
H COSMOS1			
I SYVAC/SU	1.5850E-05	9.5760E-06	3.8990E-06
J PROPER	1.5860E-05	9.7040E-06	3.9540E-06
K ESP			
L LISA4-JRC	1.5850E-05	9.5820E-06	3.9090E-06
N SYVAC3-LE1	1.5930E-05	9.6050E-06	3.9230E-06

Table B2.1 I^{129} Peak Flux (mols/yr) and Time (yrs) of Peak from Layer 1

Participant	Case 1		Case 2		Case 3	
	Flux	Time	Flux	Time	Flux	Time
A EXACT	0.1061	955	1.1690E-02	11000	4.1400E-03	49100
B LISA.SCK-4.0	0.1077	991	1.2310E-02	11500	4.5580E-03	49500
C SYVACD1000						
D SYVACD10000	0.1119	901	1.1680E-02	10100	4.7200E-03	48100
E MASCOT1000	0.1061	950	1.1690E-02	11000	4.1400E-03	49000
F MASCOT4000	0.1061	950	1.1690E-02	11000	4.1400E-03	49000
G JAERI-LHS1.1	0.1053	1000	1.1690E-02	11000	4.1220E-03	50000
H COSMOS1	0.1683	900	1.3530E-02	10900	6.5490E-03	49000
I SYVAC/SU	0.1053	1000	1.1120E-02	10000	4.1170E-03	50100
J PROPER	0.1060	971	1.1630E-02	11300	4.1260E-03	48300
K ESP	0.1002	975	1.1320E-02	11000	3.9810E-03	48800
L LISA4-JRC	0.1048	929	1.1740E-02	11200	4.1450E-03	49400
N SYVAC3-LE1	0.1062	954	1.1700E-02	11080	4.1440E-03	49010

Table B2.2 Np^{237} Peak Flux (mols/yr) and Time (yrs) of Peak from Layer 1

Participant	Case 1		Case 2		Case 3	
	Flux	Time	Flux	Time	Flux	Time
A EXACT	2.5180E-03	3.0700E+05	3.2170E-04	1.9200E+06	2.5260E-06	1.1700E+07
B LISA.SCK-4.0	2.5610E-03	3.1600E+05	3.3450E-04	1.9900E+06	2.4960E-06	1.2000E+07
C SYVACD1000	2.4350E-03	3.0600E+05	3.1310E-04	1.9000E+06	2.4420E-06	1.1500E+07
D SYVACD10000	2.4350E-03	3.0600E+05	3.1310E-04	1.9000E+06	2.4420E-06	1.1500E+07
E MASCOT1000	2.5170E-03	3.1000E+05	3.2150E-04	1.9000E+06	2.4940E-06	1.2000E+07
F MASCOT4000	2.5170E-03	3.1000E+05	3.2150E-04	1.9000E+06	2.4940E-06	1.2000E+07
G JAERI-LHS1.1	2.5150E-03	3.0000E+05	3.2150E-04	1.9000E+06	2.5260E-06	1.1600E+07
H COSMOS1						
I SYVAC/SU	2.5120E-03	3.1600E+05	3.1920E-04	2.0000E+06	2.3150E-06	1.2600E+07
J PROPER	2.5080E-03	3.1900E+05	3.2170E-04	1.9200E+06	2.5080E-06	1.1400E+07
K ESP	2.4640E-03	3.1100E+05	2.8380E-04	1.9900E+06	1.9460E-06	1.2900E+07
L LISA4-JRC	2.4770E-03	3.2400E+05	3.0400E-04	2.0100E+06	2.3630E-06	1.2200E+07
N SYVAC3-LE1	2.5180E-03	3.0810E+05	3.2180E-04	1.9250E+06	2.5270E-06	1.1620E+07

Table B2.3 U^{233} Peak Flux (mols/yr) and Time (yrs) of Peak from Layer 1

Participant	Case 1		Case 2		Case 3	
	Flux	Time	Flux	Time	Flux	Time
A EXACT	6.9520E-04	5.2400E+04	1.4770E-04	1.1200E+06	3.1390E-06	9.1700E+06
B LISA.SCK-4.0	6.9930E-04	5.0200E+04	1.4730E-04	1.2600E+06	2.9850E-06	8.5200E+06
C SYVACD1000	7.0020E-04	4.9600E+04	1.4460E-04	1.1000E+06	3.0050E-06	9.1500E+06
D SYVACD10000	7.0020E-04	4.9600E+04	1.4460E-04	1.1000E+06	3.0050E-06	9.1500E+06
E MASCOT1000	6.9510E-04	5.3000E+04	1.4770E-04	1.1000E+06	3.1380E-06	9.2000E+06
F MASCOT4000	6.9510E-04	5.3000E+04	1.4770E-04	1.1000E+06	3.1380E-06	9.2000E+06
G JAERI-LHS1.1	6.8590E-04	6.0000E+04	1.4770E-04	1.1000E+06	3.1380E-06	9.2000E+06
H COSMOS1						
I SYVAC/SU	6.9410E-04	5.0100E+04	1.4680E-04	1.0000E+06	3.0300E-06	1.0000E+07
J PROPER	6.9420E-04	4.9400E+04	1.4750E-04	1.1300E+06	3.1490E-06	9.2800E+06
K ESP	6.9270E-04	5.3500E+04	1.4540E-04	1.1000E+06	3.0060E-06	9.6400E+06
L LISA4-JRC	7.0260E-04	5.6800E+04	1.4040E-04	1.1800E+06	3.0180E-06	9.4300E+06
N SYVAC3-LE1	6.9460E-04	5.4300E+04	1.4780E-04	1.1310E+06	3.1400E-06	9.1780E+06

Table B2.4 Th^{229} Peak Flux (mols/yr) and Time (yrs) of Peak from Layer 1

Participant	Case 1		Case 2		Case 3	
	Flux	Time	Flux	Time	Flux	Time
A EXACT	3.1220E-06	6.6300E+04	6.8600E-07	1.1200E+06	1.4580E-08	9.1700E+06
B LISA.SCK-4.0	3.1260E-06	7.0900E+04	6.8390E-07	1.2600E+06	1.3870E-08	8.5200E+06
C SYVACD1000	1.8500E-06	7.2000E+04	6.8610E-07	1.1000E+06	1.4260E-08	9.1700E+06
D SYVACD10000	1.8500E-06	7.2000E+04	6.8610E-07	1.1000E+06	1.4260E-08	9.1700E+06
E MASCOT1000	3.1220E-06	6.6000E+04	6.8570E-07	1.1000E+06	1.4580E-08	9.2000E+06
F MASCOT4000	3.1220E-06	6.6000E+04	6.8570E-07	1.1000E+06	1.4580E-08	9.2000E+06
G JAERI-LHS1.1	3.0910E-06	6.0000E+04	6.8430E-07	1.1000E+06	1.4580E-08	9.2000E+06
H COSMOS1						
I SYVAC/SU	1.7860E-06	7.9400E+04	6.7270E-07	1.2600E+06	1.4070E-08	1.0000E+07
J PROPER	3.1950E-06	6.4300E+04	6.8650E-07	1.1300E+06	1.4610E-08	9.2800E+06
K ESP	3.0990E-06	6.8600E+04	6.7490E-07	1.1700E+06	1.3940E-08	9.6400E+06
L LISA4-JRC	3.1000E-06	7.3100E+04	6.5170E-07	1.1800E+06	1.4020E-08	9.5900E+06
N SYVAC3-LE1	3.1170E-06	6.8890E+04	6.8620E-07	1.1420E+06	1.4550E-08	8.9670E+06

Table B3.1 I^{129} Peak Dose (Sv/yr) and Time (yrs) of Peak

Participant	Case 1		Case 2		Case 3	
	Flux	Time	Flux	Time	Flux	Time
A EXACT	1.2180E-05	1470.	3.4850E-07	2.1000E+04	3.3230E-08	1.0800E+05
B LISA.SCK-4.0	1.2500E-05	1510.	3.6510E-07	2.2700E+04	3.4610E-08	1.0900E+05
C SYVACD1000						
D SYVACD10000	1.2150E-05	1470.	3.4810E-07	2.2100E+04	3.2750E-08	1.0600E+05
E MASCOT1000	1.2150E-05	1500.	3.4850E-07	2.1000E+04	3.3010E-08	1.1000E+05
F MASCOT4000	1.2150E-05	1500.	3.4850E-07	2.1000E+04	3.3010E-08	1.1000E+05
G JAERI-LHS1.1	1.2160E-05	1500.	3.4850E-07	2.1000E+04	3.3340E-08	1.1000E+05
H COSMOS1	1.9300E-05	1400.	4.0300E-07	2.1000E+04	5.2600E-08	1.0800E+05
I SYVAC/SU	1.1590E-05	1580.	3.2820E-07	2.0000E+04	2.7510E-08	1.0000E+05
J PROPER	1.2170E-05	1450.	3.4600E-07	2.1600E+04	3.3260E-08	1.0900E+05
K ESP	1.1760E-05	1450.	3.4600E-07	2.0500E+04	3.2800E-08	1.0600E+05
L LISA4-JRC	1.2130E-05	1500.	3.5150E-07	2.1200E+04	3.3240E-08	1.0800E+05
N SYVAC3-LE1	1.2170E-05	1494.	3.4880E-07	2.0960E+04	3.3240E-08	1.0780E+05

Table B3.2 Np^{237} Peak Dose (Sv/yr) and Time (yrs) of Peak

Participant	Case 1		Case 2		Case 3	
	Flux	Time	Flux	Time	Flux	Time
A EXACT	3.5350E-05	4.6200E+05	3.2190E-07	4.8600E+06	2.5920E-11	2.4500E+07
B LISA.SCK-4.0	3.5810E-05	4.4700E+05	3.3730E-07	5.0100E+06	2.3760E-11	2.6700E+07
C SYVACD1000	3.5140E-05	4.6300E+05	3.1420E-07	4.8500E+06	2.4050E-11	2.4600E+07
D SYVACD10000	3.5140E-05	4.6300E+05	3.1420E-07	4.8500E+06	2.4050E-11	2.4600E+07
E MASCOT1000	3.5340E-05	4.6000E+05	3.2160E-07	4.9000E+06	2.5680E-11	2.5000E+07
F MASCOT4000	3.5340E-05	4.6000E+05	3.2160E-07	4.9000E+06	2.5680E-11	2.5000E+07
G JAERI-LHS1.1	3.5340E-05	4.6000E+05	3.2170E-07	4.8000E+06	2.5850E-11	2.4500E+07
H COSMOS1						
I SYVAC/SU	3.3770E-05	5.0100E+05	3.1470E-07	5.0100E+06	2.4460E-11	2.5100E+07
J PROPER	3.5330E-05	4.5000E+05	3.2190E-07	4.8600E+06	2.5940E-11	2.4500E+07
K ESP	3.5290E-05	4.5300E+05	3.1580E-07	4.7500E+06	2.3890E-11	2.4500E+07
L LISA4-JRC	3.4770E-05	4.7700E+05	3.0170E-07	5.0200E+06	2.4230E-11	2.5400E+07
N SYVAC3-LE1	3.5310E-05	4.6830E+05	3.2190E-07	4.8350E+06	2.5930E-11	2.4580E+07

Table B3.3 U^{233} Peak Dose (Sv/yr) and Time (yrs) of Peak

Participant	Case 1		Case 2		Case 3	
	Flux	Time	Flux	Time	Flux	Time
A EXACT	9.2090E-06	6.9500E+04	2.0720E-07	3.4300E+06	3.5960E-11	2.1200E+07
B LISA.SCK-4.0	9.2940E-06	7.0900E+04	2.0630E-07	3.5500E+06	3.1840E-11	2.1300E+07
C SYVACD1000	9.9560E-06	6.7600E+04	2.0170E-07	3.4500E+06	3.2800E-11	2.1300E+07
D SYVACD10000	9.9560E-06	6.7600E+04	2.0170E-07	3.4500E+06	3.2800E-11	2.1300E+07
E MASCOT1000	9.2070E-06	6.9000E+04	2.0720E-07	3.4000E+06	3.5930E-11	2.1000E+07
F MASCOT4000	9.2070E-06	6.9000E+04	2.0720E-07	3.4000E+06	3.5930E-11	2.1000E+07
G JAERI-LHS1.1	9.0010E-06	8.0000E+04	2.0730E-07	3.4000E+06	3.5750E-11	2.1000E+07
H COSMOS1						
I SYVAC/SU	9.0160E-06	6.3100E+04	2.0670E-07	3.1600E+06	3.4230E-11	2.0000E+07
J PROPER	8.7160E-06	7.2300E+04	2.1090E-07	3.5200E+06	3.5930E-11	2.2000E+07
K ESP	8.8190E-06	7.5100E+04	2.0480E-07	3.3000E+06	3.5430E-11	2.0700E+07
L LISA4-JRC	9.3020E-06	7.3100E+04	1.9730E-07	3.5200E+06	3.4810E-11	2.1900E+07
N SYVAC3-LE1	9.1730E-06	7.2850E+04	2.0750E-07	3.3880E+06	3.5980E-11	2.1170E+07

Table B3.4 Th^{229} Peak Dose (Sv/yr) and Time (yrs) of Peak

Participant	Case 1		Case 2		Case 3	
	Flux	Time	Flux	Time	Flux	Time
A EXACT	1.2650E-05	8.3300E+04	2.9370E-07	3.4300E+06	5.0950E-11	2.1200E+07
B LISA.SCK-4.0	1.2750E-05	7.9500E+04	2.9230E-07	3.5500E+06	4.3700E-11	2.1300E+07
C SYVACD1000	1.3200E-05	8.1100E+04	2.8430E-07	3.4500E+06	4.7380E-11	2.1300E+07
D SYVACD10000	1.3200E-05	8.1100E+04	2.8430E-07	3.4500E+06	4.7380E-11	2.1300E+07
E MASCOT1000	1.2650E-05	8.3000E+04	2.9370E-07	3.4000E+06	5.0920E-11	2.1000E+07
F MASCOT4000	1.2650E-05	8.3000E+04	2.9370E-07	3.4000E+06	5.0920E-11	2.1000E+07
G JAERI-LHS1.1	1.2640E-05	8.0000E+04	2.9370E-07	3.4000E+06	5.0650E-11	2.1000E+07
H COSMOS1						
I SYVAC/SU	1.2550E-05	7.9400E+04	2.7590E-07	3.9800E+06	4.8270E-11	2.0000E+07
J PROPER	1.2980E-05	9.2800E+04	2.9780E-07	3.5200E+06	5.0920E-11	2.2000E+07
K ESP	1.2620E-05	8.4200E+04	2.9020E-07	3.3000E+06	5.0210E-11	2.0900E+07
L LISA4-JRC	1.2490E-05	9.1300E+04	2.7950E-07	3.5900E+06	4.9320E-11	2.2100E+07
N SYVAC3-LE1	1.2640E-05	8.2520E+04	2.9400E-07	3.3800E+06	5.0970E-11	2.1280E+07

Table C1.1 I^{129} Mean Dose (Sv/yr) at Given Times (yrs)

Participant	1×10^4	2×10^4	5×10^4	1×10^5	2×10^5	5×10^5
A EXACT	3.7790E-08	7.8540E-08	5.3820E-08	2.3530E-08	9.9810E-09	2.8220E-09
B LISA.SCK-4.0	2.5100E-08	6.5370E-08	5.9140E-08	2.5510E-08	1.1500E-08	1.5880E-09
C SYVACD1000						
D SYVACD10000	3.2320E-08	6.9940E-08	4.6180E-08	2.1790E-08	8.5580E-09	
E MASCOT1000	3.2040E-08	7.5830E-08	5.8660E-08	2.4360E-08	7.9760E-09	2.9510E-09
F MASCOT4000	3.8940E-08	7.5900E-08	5.4120E-08	2.2360E-08	1.0470E-08	2.9620E-09
G JAERI-LHS1.1	3.6330E-08	7.6580E-08	5.3470E-08	2.3330E-08	1.0030E-08	2.9320E-09
H COSMOS1	1.0320E-07	2.4310E-07	2.0510E-07	7.1070E-08	2.2430E-08	5.8180E-09
I SYVAC/SU	4.6600E-08	9.5780E-08	4.8430E-08	2.3550E-08	1.1140E-08	2.3730E-09
J PROPER	4.7600E-08	7.6370E-08	6.7300E-08	2.7430E-08	9.2490E-09	5.4890E-09
K ESP	3.2200E-08	6.8900E-08	4.9800E-08	2.5300E-08	9.9900E-09	2.7300E-09
L LISA4-JRC	4.9140E-08	9.7700E-08	5.1080E-08	2.5960E-08	8.1540E-09	2.0950E-09
N SYVAC3-LE1	5.8420E-08	9.7200E-08	5.0490E-08	2.8690E-08	9.0850E-09	3.6790E-09

Table C1.2 I^{129} Standard Deviation (Sv/yr) at Given Times (yrs)

Participant	1×10^4	2×10^4	5×10^4	1×10^5	2×10^5	5×10^5
A EXACT						
B LISA.SCK-4.0	1.5520E-07	3.0340E-07	1.7760E-07	9.7720E-08	3.9650E-08	6.8050E-09
C SYVACD1000						
D SYVACD10000	2.5710E-07	3.0990E-07	1.4730E-07	6.4200E-08	2.9500E-08	
E MASCOT1000	2.4510E-07	3.0700E-07	1.8050E-07	7.1960E-08	2.6770E-08	1.0330E-08
F MASCOT4000	3.0910E-07	3.2470E-07	1.6250E-07	7.0230E-08	3.5190E-08	1.2160E-08
G JAERI-LHS1.1	2.6430E-07	3.0320E-07	1.6730E-07	7.7950E-08	4.2360E-08	1.5920E-08
H COSMOS1	1.0440E-06	1.0940E-06	6.7010E-07	2.4340E-07	8.0880E-08	2.4900E-08
I SYVAC/SU	3.6730E-07	3.4750E-07	1.3430E-07	6.9580E-08	3.8650E-08	1.0730E-08
J PROPER	3.8820E-07	3.3940E-07	2.3220E-07	9.7340E-08	3.7510E-08	4.2810E-08
K ESP	2.1800E-07	1.8500E-07	1.0000E-07	4.8500E-08	2.1300E-08	7.7400E-09
L LISA4-JRC	3.7630E-07	4.0900E-07	1.6880E-07	8.5610E-08	2.9730E-08	1.0440E-08
N SYVAC3-LE1	4.4600E-07	3.8110E-07	1.4410E-07	8.5670E-08	2.9730E-08	1.3920E-08

Table C2.1 I^{129} Mean of Maximum Dose (Sv/yr) up to Given Times (yrs)

Participant	1×10^4	2×10^4	5×10^4	1×10^5	2×10^5	5×10^5
A EXACT						
B LISA.SCK-4.0						
C SYVACD1000						
D SYVACD10000	4.2850E-08	1.4550E-07	2.4620E-07	2.7790E-07	2.9020E-07	
E MASCOT1000	3.3680E-08	1.2600E-07	2.2810E-07	2.6650E-07	2.7710E-07	2.8260E-07
F MASCOT4000	4.4710E-08	1.3570E-07	2.3660E-07	2.6770E-07	2.8040E-07	2.8580E-07
G JAERI-LHS1.1	4.2920E-08	1.4080E-07	2.5090E-07	2.8060E-07	3.0220E-07	3.1110E-07
H COSMOS1						
I SYVAC/SU	6.2020E-08	1.6700E-07	2.6620E-07	2.9650E-07	3.0890E-07	3.1400E-07
J PROPER	4.9510E-08	1.4560E-07	2.7450E-07	3.3190E-07	3.5660E-07	3.8640E-07
K ESP	4.9000E-08	1.1000E-07	2.0700E-07	2.4300E-07	2.5000E-07	2.5400E-07
L LISA4-JRC	5.9300E-08	1.7450E-07	2.7410E-07	3.1230E-07	3.2250E-07	3.2770E-07
N SYVAC3-LE1	7.9310E-08	1.9620E-07	3.0750E-07	3.4740E-07	3.5950E-07	3.6590E-07

Table C2.2 I^{129} Standard Deviation of Maximum Dose (Sv/yr) up to Given Times (yrs)

Participant	1×10^4	2×10^4	5×10^4	1×10^5	2×10^5	5×10^5
A EXACT						
B LISA.SCK-4.0						
C SYVACD1000						
D SYVACD10000	1.1170E-07	1.9340E-07	2.1190E-07	2.1190E-07	2.1080E-07	
E MASCOT1000	2.5740E-07	4.9990E-07	5.6420E-07	5.6910E-07	5.6620E-07	5.6400E-07
F MASCOT4000	3.8280E-07	5.7070E-07	6.2910E-07	6.2910E-07	6.2580E-07	6.2350E-07
G JAERI-LHS1.1	3.2960E-07	5.5590E-07	6.3440E-07	6.3830E-07	6.3360E-07	6.3080E-07
H COSMOS1						
I SYVAC/SU	5.1860E-07	6.4200E-07	6.9190E-07	6.9000E-07	6.8660E-07	6.8470E-07
J PROPER	3.9390E-07	6.2900E-07	7.2110E-07	7.6820E-07	7.6530E-07	7.6290E-07
K ESP	4.0800E-07	4.7200E-07	5.4200E-07	5.4600E-07	5.4400E-07	5.4200E-07
L LISA4-JRC	4.1980E-07	6.7650E-07	7.2570E-07	7.2660E-07	7.2390E-07	7.2200E-07
N SYVAC3-LE1	5.8650E-07	7.6960E-07	8.2490E-07	8.2370E-07	8.2050E-07	8.1810E-07

Table C3.1 Total Dose (Sv/yr) at Given Times (yrs)

Participant	5×10^5	1×10^6	2×10^6	5×10^6	1×10^7
A EXACT	2.7620E-08	4.9050E-08	6.5060E-08	6.4750E-08	1.8450E-08
B LISA.SCK-4.0	1.8070E-08	3.6690E-08	5.0960E-08	6.4400E-08	1.7800E-08
C SYVACD1000		5.3470E-08	6.7270E-08	6.7330E-08	1.7550E-08
D SYVACD10000		5.6880E-08	7.1390E-08	7.0790E-08	1.8250E-08
E MASCOT1000	1.2110E-08	3.3760E-08	4.4900E-08	5.8230E-08	1.7590E-08
F MASCOT4000	2.5380E-08	4.7640E-08	6.2990E-08	6.7330E-08	1.7170E-08
G JAERI-LHS1.1	2.7600E-08	4.8150E-08	6.4630E-08	6.6040E-08	1.7810E-08
H COSMOS1					
I SYVAC/SU	2.5420E-08	4.1020E-08	6.6060E-08	5.4290E-08	2.2390E-08
J PROPER	2.4890E-08	3.8010E-08	7.5840E-08	4.6780E-08	1.6560E-08
K ESP	1.5400E-08	3.5500E-08	4.9100E-08	6.0600E-08	2.1700E-08
L LISA4-JRC	2.4590E-08	4.7600E-08	6.4320E-08	6.7060E-08	1.7410E-08
N SYVAC3-LE1	1.8290E-08	4.0690E-08	5.5340E-08	8.0420E-08	2.4240E-08

Table C3.2 Standard Deviation of Dose (Sv/yr) at Given Times (yrs)

Participant	5×10^5	1×10^6	2×10^6	5×10^6	1×10^7
A EXACT					
B LISA.SCK-4.0	1.1660E-07	1.9190E-07	2.4500E-07	3.4940E-07	6.1320E-08
C SYVACD1000		1.5000E-07	1.5000E-07	1.5000E-07	4.4000E-08
D SYVACD10000		1.3060E-07	1.6160E-07	1.1840E-07	2.1500E-08
E MASCOT1000	1.0740E-07	1.8450E-07	2.3810E-07	2.9620E-07	6.5230E-08
F MASCOT4000	2.8310E-07	3.3670E-07	4.8180E-07	3.4810E-07	6.5070E-08
G JAERI-LHS1.1	2.8310E-07	3.1680E-07	4.3660E-07	3.3910E-07	6.5470E-08
H COSMOS1					
I SYVAC/SU	2.8120E-07	3.1000E-07	5.2020E-07	2.7930E-07	7.5650E-08
J PROPER	2.9430E-07	2.3520E-07	6.7450E-07	2.1700E-07	7.4870E-08
K ESP	9.7600E-08	1.8600E-07	2.2400E-07	3.1300E-07	5.2000E-08
L LISA4-JRC	2.1530E-07	2.7550E-07	3.6550E-07	3.1950E-07	6.2380E-08
N SYVAC3-LE1	1.2630E-07	2.3160E-07	2.8420E-07	4.1880E-07	7.6730E-08

Table C4.1 Mean of Maximum Dose (Sv/yr) from Chain up to Given Times (yrs)

Participant	5×10^5	1×10^6	2×10^6	5×10^6	1×10^7
A EXACT					
B LISA.SCK-4.0					
C SYVACD1000		5.6260E-08	6.7700E-08	9.5640E-08	1.0640E-07
D SYVACD10000		5.6260E-08	6.7700E-08	9.5640E-08	1.0640E-07
E MASCOT1000	1.2160E-08	3.4050E-08	4.4950E-08	7.1400E-08	7.9840E-08
F MASCOT4000	2.5510E-08	4.9140E-08	6.3180E-08	9.4030E-08	1.0260E-07
G JAERI-LHS1.1	2.7600E-08	4.9500E-08	6.4910E-08	9.5700E-08	1.0440E-07
H COSMOS1					
I SYVAC/SU	2.7780E-08	4.3260E-08	6.9620E-08	1.0810E-07	1.2130E-07
J PROPER	3.2540E-08	7.5880E-08	1.1420E-07	1.4300E-07	1.4810E-07
K ESP	1.5500E-08	3.5800E-08	4.9100E-08	7.3100E-08	8.2700E-08
L LISA4-JRC	2.4670E-08	4.9170E-08	6.4610E-08	9.6440E-08	1.0460E-07
N SYVAC3-LE1	1.8320E-08	4.0960E-08	5.5390E-08	8.9690E-08	1.0150E-07

Table C4.2 Standard Deviation of Maximum Dose (Sv/yr) from Chain up to Given Times (yrs)

Participant	5×10^5	1×10^6	2×10^6	5×10^6	1×10^7
A EXACT					
B LISA.SCK-4.0					
C SYVACD1000		1.2980E-07	1.4810E-07	1.9690E-07	2.0410E-07
D SYVACD10000		1.2980E-07	1.4810E-07	1.9690E-07	2.0410E-07
E MASCOT1000	1.0750E-07	1.8610E-07	2.3830E-07	3.8060E-07	3.9080E-07
F MASCOT4000	2.8560E-07	3.5350E-07	4.8270E-07	6.3770E-07	6.4410E-07
G JAERI-LHS1.1	2.8310E-07	3.3480E-07	4.3850E-07	5.6650E-07	5.7280E-07
H COSMOS1					
I SYVAC/SU	3.1280E-07	3.3880E-07	5.7530E-07	7.7020E-07	7.7440E-07
J PROPER	4.1550E-07	8.9060E-07	1.0200E-06	1.0580E-06	1.0600E-06
K ESP	1.1400E-07	2.2100E-07	2.7300E-07	4.1500E-07	4.2300E-07
L LISA4-JRC	2.1580E-07	2.8840E-07	3.6710E-07	5.1320E-07	5.2030E-07
N SYVAC3-LE1	1.2630E-07	2.3220E-07	2.8430E-07	4.6840E-07	4.8060E-07

AVAILABILITY OF COMPUTER CODES

Of the computer programs used in this study, two had been released to the NEA Data Bank for distribution within the PSAC User Group at the time of writing of this report: LISA4-JRC and SYVAC-D. These codes are available under certain conditions to users who are not members of the PSAC User Group. For more information, write to

NEA Data Bank
Bâtiment 445
91191 Gif-sur-Yvette Cedex
France

Some of the computer codes used in this study have not yet been released for general distribution, the main reason being that they are still under development. For specific questions concerning particular computer codes, including when they may be available for release, the reader should refer to the contact persons listed in Annex B of this report.

References

Chatfield, C. and Collins, A.J., 1983. Introduction to Multivariate Analysis. Chapman and Hall, London.

Hogg, R.V. and Craig, A.T., 1978. Introduction to Mathematical Statistics. MacMillan Publishing Co. (U.S.A.), 4th Edition, p. 204.

McCay, M.D., Beckman, R.J. and Conover, W.J., 1979. A comparison of three methods for selecting values of input variables in the analysis of output from a computer code. Technometrics, 21(2), p. 239.

NEA PSAC User Group, 1987. PSACOIN Level 0 Intercomparison. Edited by A. Saltelli, E. Sartori, T.H. Andres, B.W. Goodwin and S.G. Carlyle. NEA/OECD, Paris.

Oldfield, S., Sinclair, J., Andres, T. and Robinson, P., 1988. PSACOIN Level E Intercomparison Case Specification. PSAC/DOC(87)13, NEA/OECD, Paris.

Robinson, P., 1988. The Mathematical Basis for the Exact Results used in the NEA PSAC User Group Level E Intercomparison Exercise. Intera/ECL Report I1901-2, Issue 1.

Robinson, P. and Hodgkinson, D., 1987. Exact solutions for radionuclide transport in the presence of parameter uncertainty. Rad. Waste Mngmt. and the Nuc. Fuel Cycle, 8(4), p. 283.

Saltelli, A. and Marivoet, J., 1988. Safety assessment for nuclear waste disposal: some observations about actual risk calculations. Rad. Waste Mngmt. and the Nuc. Fuel Cycle, 9(4), p. 309.

SAS Institute Inc., 1985. SAS User's Guide: Statistics. SAS Institute Inc., Cary, NC, Version 5.

Talbot, A., 1979. The accurate numerical inversion of Laplace transforms. J. Inst. Math. Appl., 23, p. 97.

Woo, G., 1989. Confidence bounds on risk assessments for underground nuclear waste repositories. Terra Nova, 1(1), p. 79.

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This report describes an international code intercomparison exercise conducted by the NEA Probabilistic System Assessment Code (PSAC) User Group. Termed PSACOIN Level E, it is the second of a series designed to contribute to the verification of probabilistic codes that may be used in assessing the safety of radioactive waste disposal systems or concepts. The principal aim of this exercise was to test the basic functions of each code by using a system model describing a hypothetical disposal concept for which there was an "exact" analytical solution (hence Level "E"). The report compares results, provides recommendations on procedures for future intercomparison exercises, and concludes that most codes are functioning as intended and meet their design requirements.