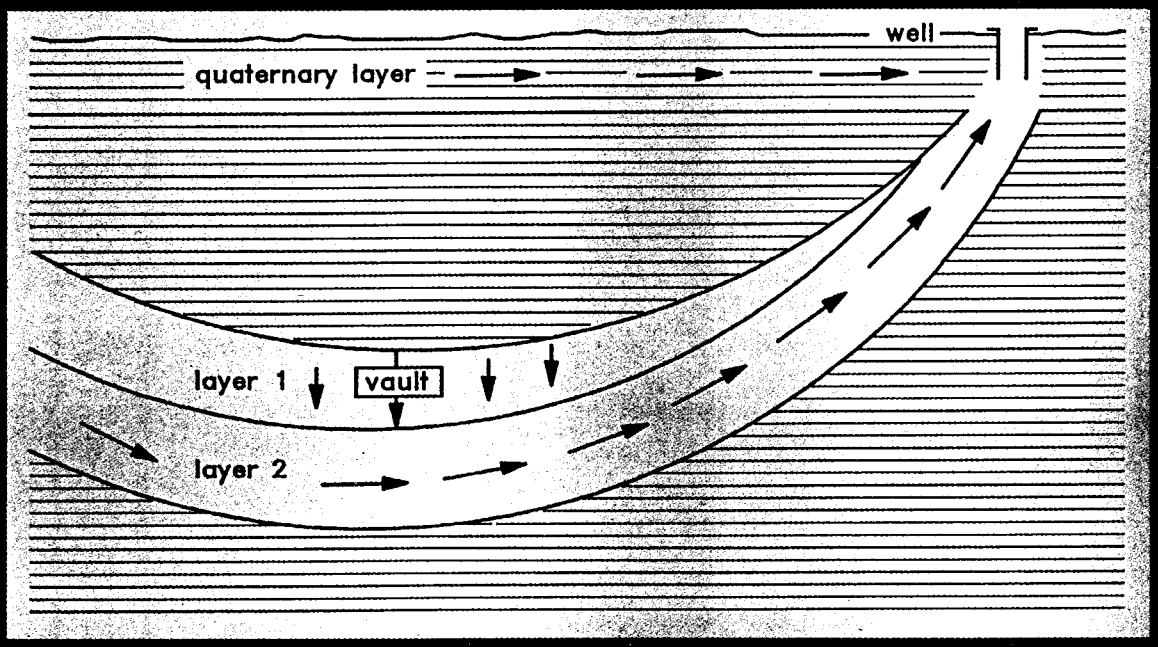
An International Code Intercomparison Exercise
on a Hypothetical Safety Assessment Case Study
for Radioactive Waste Disposal Systems

PSACOIN LEVEL 1A INTERCOMPARISON

Probabilistic System Assessment Code (PSAC) User Group



NUCLEAR ENERGY AGENCY

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Probabilistic System Assessment Code (PSAC) User Group

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

The NEA Probabilistic System Assessment Code (PSAC) User Group was established by the RWMC in January 1985 to help coordinate 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. This is the third in a planned series of code intercomparisons undertaken by the Group and published by the OECD/NEA.

The NEA Data Bank undertakes the collection, validation, and dissemination of computer programmes and scientific data within the NEA's field of interest. Among its tasks is the provision of computing support for radioactive waste management activities, including code exchange and the analysis of code intercomparisons.

CONTENTS

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This report includes case studies from each of the individuals listed above. The conclusions and recommendations presented here are 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 comprehensible results when applied to the same problem. Such evidence contributes to the verification of the codes involved.

This report documents the Group's third PSA code intercomparison (PSACOIN) exercise, known as Level 1a. This exercise is a direct succession to the Level 0 and Level E exercises. Level 0 involved a relatively simple disposal system model, and code verification focused on the executive and postprocessing functions. In Level E, the existence of an "exact" analytical solution was particularly important because it allowed not only intercomparison of the results between codes, but also a benchmark against which the results from all codes could be compared.

Level 1a represents a step toward an intercomparison based on a more realistic system model - in this case, involving deep geological disposal concepts with a relatively complex structure of the repository vault. Radionuclides released from the repository vault were assumed to be transported by groundwater through two geosphere layers with different hydrogeological properties. Radionuclides leaving the geosphere were assumed to enter a well from which the critical group obtains drinking water. Dilution within the system was considered to occur by mixing of groundwater from a deep aquifer with that from a shallow aquifer at the source of the well. The radionuclide flow paths through the geosphere and biosphere were, therefore, described in detail. The radionuclide inventory, geometry, and physical and chemical properties of the repository were also described in detail. The overall consequence values - dose rate to a member of the critical group as a function of time - were obtained by simulating radionuclide releases from the repository, transport through two geosphere layers, and dilution and exposure in the biosphere.

In addition to the general purpose of all PSACOIN exercises of contributing to code verification, the Level La exercise had two principal objectives:

(1) The primary purpose of the exercise was to begin to evaluate the magnitude of the differences arising from the use of different mathematical approaches to modelling a set of given processes expected to be of importance in the safety assessment of radioactive waste disposal, and to weigh these differences against the variations arising from (specified) uncertainties in the input data. This represents a contrast to previous exercises, in which the system model was completely specified and differences in deterministic results were primarily due to different coding techniques, and differences in stochastic results to coding and data sampling techniques, as well as to natural statistical variation.

(2) A second purpose was to provide an indication of the possible importance to safety of various processes within and around a deep geological repository.

The main conclusions which have been drawn from this study can be summarised as follows:

- With one exception, times of peak dose, as calculated by participants for the three deterministic cases, are in excellent agreement with each other - generally within 10% of the mean value.

- The bulk of results for peak dose rates show good agreement; the range of values generally varies over an order of magnitude. Given the level of freedom in modelling the case, this level of agreement is encouraging. In many cases, individual discrepancies could be attributed to different modelling approaches.

- Different assumptions were made mainly in modelling radionuclide releases out of the repository vault and dilution of contaminated flow during transit to the biosphere. In the context of this exercise, there are combinations of input parameter values for which diffusion significantly contributes to total release from the repository. Although differences in the representation of diffusion from the repository contributed to differences in results, the concurrent use of different assumptions to model other processes - particularly dilution - makes the interpretation of such differences in results difficult. In contrast, differences in calculated radionuclide release rates from the repository could not be correlated with different approaches to representing solubility limitation.

- Under the conditions of the exercise, it was found that the variability in results attributable to data uncertainty was generally at least twice as great as that attributable to the different modelling approaches used by the participants. It is recognised, however, that the design of the case and the codes available to the participants probably limited the extent to which model uncertainty could be addressed. In addition, further thought is needed on the methodology for comparison of uncertainties arising from the two sources.

As noted above, the Level 1a exercise was a first step in estimating the relative importance of model uncertainties and data variability. The results from this limited study should, however, be interpreted with care. The case specification was such as to limit the range of modelling approaches that could be adopted, with a view to ensuring that the results obtained would be generally interpretable. Also, the constraints imposed in the case specification meant that some of the models were being used outside their stated domain of applicability, resulting in considerable effort being required by some participants to configure their models to meet the specification and to interpret the results obtained. Finally, the ranges of variability of the parameters were arbitrarily set and, for many parameters, the variability assigned was relatively large.

Future PSACOIN exercises should study in more detail the importance of modelling uncertainty relative to that arising from the variability of input data. In particular, it is considered that the case specifications should allow participants greater scope to adopt alternative modelling approaches.

1. GENERAL INTRODUCTION

1.1 Background

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 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 third PSA code intercomparison (PSACOIN) exercise, known as Level 1a. This exercise is a direct succession to the Level 0 [1] and Level E [2] exercises. Level 0 involved a relatively simple disposal system model, and code verification focused on the executive and postprocessing functions. In Level E, the existence of an "exact" analytical solution was particularly important because it allowed not only intercomparison of the results between codes, but also a benchmark against which the results from all codes could be compared.

Level 1a represents a step toward an intercomparison based on a more realistic system model - in this case, involving deep geological disposal concepts with a relatively complex structure of the repository vault. Other PSACOIN studies in progress include Level S - an intercomparison of different techniques for sensitivity analysis, based on the Level E exercise - and Level 1b - a test of more detailed biosphere submodels, using a system model that may be considered to represent certain near-surface disposal concepts. Further studies are being discussed within the PSAC User Group, and such "Level 2" studies will likely contribute further steps toward realism in PSA code intercomparisons.

1.2 Purpose of the Level 1a Exercise

In addition to the general purpose of all PSACOIN exercises of contributing to code verification, the Level 1a exercise had two principal objectives:

(1) The primary purpose of the Level 1a exercise was to examine the effects on particular code outputs of introducing different assumptions in the mathematical modelling of a hypothetical disposal system, and weigh the magnitude of these effects against the variations arising from specified uncertainties in the input data. Thus, an attempt was made to describe the disposal system in terms of geometries of the system, data and their distribution functions for physical and chemical properties, and processes to be modelled. No mathematical equations were provided in the case specification, nor were all modelling approaches specified in detail, even if some constraints were applied. For the exercise to be effective, it was intended that any changes to existing submodels should be kept to the minimum, and that production submodels should be used to the extent possible. This represents a contrast to previous exercises, in which the system model was completely specified and differences in deterministic results were largely due to different coding techniques, and differences in stochastic results to coding and data sampling techniques, as well as to natural statistical variation.

(2) A second purpose was to provide an indication of the importance to safety of various processes within and around a deep geological repository. Large variations in results attributable to different modelling of the information provided in the case study might indicate - for some disposal concepts and sites - that relatively detailed vault modelling should constitute an important part of reducing the overall uncertainties in assessment results.

1.3 Problem Specification

The detailed case specification for the Level 1a exercise is reproduced in Annex A, together with the questionnaire used to obtain results in a standard form. The Level 1a case specification was designed to represent deep geological disposal concepts in an hypothetical formation connected to a deep aquifer (Fig. 1.1). The radionuclides released from the repository vault are transported by groundwater through two geosphere layers with different hydrogeological properties. Radionuclides leaving the geosphere enter a well from which the critical group obtains drinking water. Dilution within the system is considered to occur by mixing of groundwater from a deep aquifer (geosphere layer 2) with that from a shallow aquifer at the source of the well. The radionuclide flow paths through the geosphere and biosphere are therefore described in detail. The radionuclide inventory, geometry, and physical and chemical properties of the repository are also described in detail.

The model has a total of some 100 parameters, about half of which are taken as variables sampled (randomly) from their probability distributions (except in deterministic analyses). Five single nuclides and two decay chains are considered: C-14, Ni-59, Se-79, Tc-99, I-129, and the decay chains Np-237 - U-233 - Th-229 and U-238 - U-234 - Th-230 - Ra-226 - Pb-210. The overall consequence values - dose rate to a member of the critical group as a function of time - are obtained by simulating radionuclide releases from the repository, transport through two geosphere layers, and dilution and exposure in the biosphere.

Table 1.1: List of contributions to the PSACOIN Level 1a exercise.

Letter	Code	Establishment	Country
A	EMOS4	GSF/IfT	F.R of Germany
B	JAERI-1.4	JAERI	Japan
C	LISA-1A/CI	CIEMAT	Spain
D	SIMPAR-2.0	ETSII	Spain
E	LISA-1A/JRC	JRC-Ispra	CEC
F	MASCOT-3	AEA Technology	UK
G	STRAW-1.1	AEA Technology	UK
H	SYVAC/FI	VTT	Finland
I	VANDAL-1.2C	Electrowatt/UKDOE	UK
J	(E)LISA-01	CIEMAT	Spain
K	NEFTRAN-B.2	SNL	USA
L	SYVAC3-L1A	AECL	Canada

Letter	Deterministic	Stochastic		Changes made for 2nd iteration	see note
	no. of timesteps DETRUN1/2/3	no.of runs	timesteps per run		
A	2212/500/4000	1000	548-43147	more stochastic runs	1
B		1000		new version, new results	2
C	1000 all runs	100	1000	no change	
D		100		new code, new results	3
E	1000 all runs	490	500-10000	new results	4
F		1000		no change	
G				no change	
H	500 all runs	1000	200	no change	
I	2200/1600/2000	500	variable	more stochastic runs	5
J	<=10000 all runs	120	<=10000	new participant	6
K	2000 all runs	25	2000	new participant	7
L	<=200 all runs	971	<=100	new participant	

Notes

1 Only 200 stochastic runs had been completed for the 1st iteration.
2 The code was modified, the version number increased to 1.4 and the whole analysis repeated.
3 The results for the first iteration using the code LISA-1A were preliminary and involved very few stochastic runs; the 2nd iteration results were produced using an entirely new code and they replaced the previous results.
4 All results in the 2nd iteration follow the model modifications described in Section B of the questionnaire - see Annex B.
5 Only 100 stochastic runs had been completed for the 1st iteration.
6 For the 2nd iteration this participant produced a new set of results using a modified LISA code (descibed in Section B of the questionnaire see Annex B). The original results after the 1st iteration have been retained under participant C, and the new results entered under J.
7 This code is a modified version of version B.2. The number of timesteps corresponds to a 100,000-year simulation. The following note was included in the questionnaire concerning the stochastic runs: '25 runs with 15 random variables, all Kd values were kept fixed at the values used in Deterministic Run 3 (mid-points of the pdfs) and the solubility limits were not part of the NEFTRAN model and, hence, were not used'.

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 C of the questionnaire). Results requested comprise, for each of the three simulations, radionuclide release rates from the vault at three specified times for five radionuclides, periods in which solubility limits are exceeded in the vault for three radionuclides, peak doses and times of peak for five radionuclides, and total doses from all radionuclides at specified time points. For stochastic analyses, results requested comprise estimates of the mean and standard deviation of the total dose and confidence bounds on the estimated mean dose at six specified times (Section D of the questionnaire).

1.4 Limitations of the Level 1a Exercise

Various constraints were imposed in the case specification that narrowed the possible range of modelling assumptions that might be made in a real assessment. In this sense, the Level 1a exercise should be considered a transition between the complete model inflexibility of Level E (all necessary equations are provided) and future exercises that would allow a more realistic and perhaps variable set of assumptions to be made by the participants. In particular, both the data and processes to model were specified in the exercise; in a more realistic situation, the modeller would have access to a much fuller and less precisely specified set of data, and interpretation of these data would add another layer of uncertainty to the modelling approach.

The geosphere and biosphere submodels were particularly constrained in the Level 1a exercise. For example, the characteristics of the data imply the use of a one-dimensional model. In addition, groundwater velocities in the two layers were given explicitly, which meant that geosphere submodels that calculate groundwater flow based on permeability distributions could not be used. Indeed, there is little conceptual difference in this part of the system model from that used in the Level E exercise.

The repository specification offered a greater deal of flexibility in modelling approach, but here again, the specificity of the input variables tended to limit the flexibility in modelling approach. For example, the absence of a diffusion term (see Annex A) suggests that all transport through the repository be considered as purely advective. In addition, specification of the time of failure of the waste containers (TDRUM) and of the cement matrix (TMATRIX) can be considered to impose particular material degradation models within the repository.

Another potential limitation concerns the procedure that was followed in reaching the final set of results for detailed analysis. The exercise ran for two complete iterations. For some participants one iteration was sufficient, whereas others joined the exercise only after the first iteration had been completed. The majority of participants changed their results in some way from the first to the second iteration. In some cases, these changes were simply because more stochastic runs had been completed, while other changes were due to the discovery of coding errors. Also, results may have been changed because of a different interpretation by the participant of the information provided in the case specification, usually as a result of informal discussions with other participants; such changes do not imply that the

results from the first iteration were necessarily incorrect. For one participant, results from both iterations were retained in order to assess the influence of such changes in interpretation. It should also be noted that where participants have modified their code between iterations, biases may have been introduced because the exercise was no longer being analysed "blind", and such results are not easily comparable to results from participants having completed only one iteration.

In summary, some of the limitations noted above led several participants to modify their codes or to input artificial data in order to model the case as specified. To the extent that such actions were undertaken, the exercise was unable to represent the full range of modelling approaches that might be made for a real assessment.

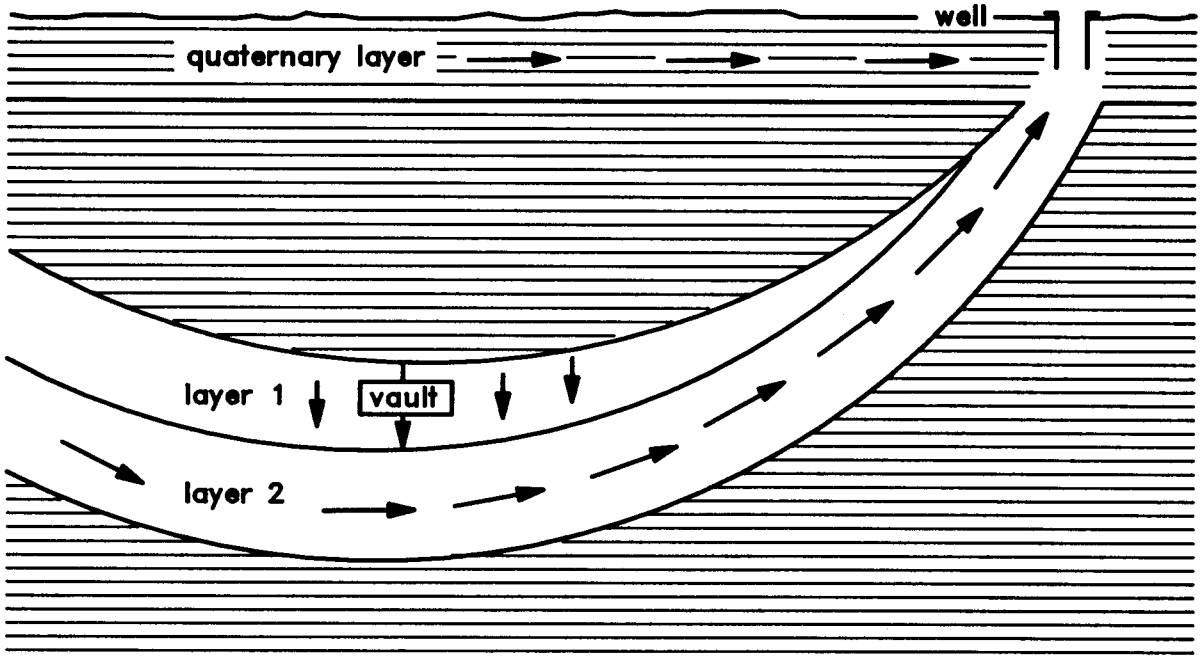
1.5 Participants

Twelve contributions were received from 10 participants (two participants submitted two results questionnaires). Table 1.1 identifies all participants, summarises the code and sample size (for stochastic runs) used, and gives an indication of the time-stepping employed. Table 1.1 also includes a unique letter for each contribution to identify it in the tables and figures provided in Sections 2 and 3 of this report.

Annex B contains descriptions of the various codes used. Particular modelling assumptions have been described in order to assist the Task Group in interpreting any differences between results. In addition, the contributions provided in Annex B have been used in preparing Sections 2 and 3 of this report.

Tables of original results from the 12 case studies contributed by participants are included as Annex C of this report. These data are also freely available in machine-readable format from the NEA Data Bank.

Fig. 1.1: Schematic illustrations of the system to be modelled in the PSACOIN Level 1a exercise. Radionuclides released from a deeply situated repository vault (with internal structure, not shown) are transported through two geosphere layers and enter a well from which the critical group obtains drinking water.



2. MODELLING APPROACHES

2.1 Introduction

As discussed in Section 1, a principal objective of the Level 1a exercise was to evaluate the relative importance of uncertainty, or bias, introduced by the use of different approaches to model the data and processes given in the case specification. The range of output arising from the use of different modelling approaches is analysed in Section 3 of the report, and this range is compared to that introduced by the (specified) uncertainty in input data. The purpose of this Section is to examine in general terms the different modelling approaches employed for the Level 1a exercise, on the basis of the information provided by participants and included in Annex B of the report and, thereby, to set the scene for the analysis presented in Section 3. A general overview of the extent to which the participants' modelling approach differed from that described in the case specification is provided in Table 2.1. This Table indicates, in qualitative terms, for each participant and for each main process, whether the model used was identical to that proposed in the specification. All deviations from the specification are discussed individually below, and the implications of these deviations are pointed out in Section 3 of the report.

2.2 Repository

The information provided in the case specification for the repository offered the most flexibility to participants in terms of modelling approach. Consequently, it was considered that differences in deterministic results would arise largely from different possible implementations of this part of the system model.

The processes to be modelled within the repository are described in detail in Section 2.2 of the case specification (Annex A):

- constant radionuclide release rate from the cement waste matrix;
- constant radionuclide release rate from the steel drums;
- precipitation of radionuclides when solubility limits are exceeded in the repository; and
- sorption of radionuclides by the cement - in the form of waste matrix and backfill material - within the repository.

Specification of this set of processes implies a series of assumptions concerning the behaviour of radionuclides within the repository and how they would be released to the surrounding medium. For example, mobilisation of radionuclides from the waste drums had to be modelled by combining releases

Table 2.1: Divergence between the case specification and the models used, as described by each participant in Annex B of the report. An "X" indicates that the process was modelled exactly as described in the specification. An "O" indicates that the participant deviated from the specification. Also, an "O" is used to indicate that the participant included an additional process (e.g., diffusion in the vault).

	PARTICIPANT											
PROCESS	A	B	C	D	E	F	G	H	I	J	K	L
VAULT												
Corrosion	X	X	X	X	X	O	O	X	X	X	O	X
Matrix degradation	X	X	X	X	X	O	O	X	O	X	O	X
Solubility limit	X	X	X	X	X	O	X	X	O	X	O	X
Transport in matrix	X	X	X	X	X	X	X	X	O	X	O	X
Additional process				O		O	O	O	O		O	O
GEOSPHERE												
Advection	X	X	X	X	X	X	O	X	X	X	X	X
Diffusion	X	X	X	X	X	X	O	X	X	X	O	X
Dispersion	X	X	X	X	X	X	O	X	O	X	X	X
Additional process									O			O
BIOSPHERE												
Dilution	X	X	X	X	X	X	O	X	O	X	X	X
Dose conversion factor	X	X	X	X	X	X	O	X	X	X	X	X

from the waste matrix, spread over time in a specified way, with releases from the drums, also spread over time in a specified way. Whereas some participants chose to write special submodels to correspond exactly to this set of assumptions, others used previously developed PSA submodels without modification, and adjusted various model inputs in an attempt to conform with these assumptions to the extent possible. Repository release submodels actually used range from much simpler to much more sophisticated than that described in the case specification. Many possible sources of discrepancy between participants' results were thereby introduced:

(1) Some submodels used required the specified constant radionuclide release rates from the engineered containment barriers to be implemented as a sudden release, at one extreme, or as a nonlinear release, at another extreme.

(2) Different approaches to vault modelling were employed, ranging from considering the entire vault as a mixing tank to detailed evaluation of advective-diffusive transport through the vault.

(3) One participant (I) assumed that radionuclide concentrations in the waste containers would generally be larger than those in the surrounding backfill and, therefore, solubility limits were only applied to radionuclide releases from the waste containers to the backfill and not for transport through the backfill to the geosphere; other participants' submodels were not based on such an assumption.

(4) Similarly, one participant (I) assumed that sorption should be modelled for releases from the waste container and for transport through the backfill; other participants considered sorption only in the backfill.

(5) Some submodels did not apply nuclide-specific solubility limits for releases from the waste containers; others did.

(6) Although the case specification did not state that diffusion should be modelled within the repository, the submodels of several participants did include diffusion within the repository. These participants had to provide their own choice of diffusion coefficients in their model implementations.

(7) The code of one participant (K) did not contain a repository submodel. Rather than modify the code to include such a submodel, this participant chose to simulate the repository by extending the transport path. The length of this extension was selected so that the radionuclide travel time through it was equal to the radionuclide residence time within the repository. This approach required that the values of some transport properties within the repository, such as dispersivity, be assigned arbitrarily.

2.3 Geosphere

All participants represented the geosphere transport, to the extent possible, as specified: one-dimensional advective-diffusive transport through two consecutive layers, with all dilution assumed to occur at the end of the second layer. There could be at least three possible sources of discrepancy between participants' results arising from the implementation of the geosphere submodel:

(1) Some submodels require continuous dilution along the flow path; the specification required participants with these submodels to introduce a correction to the dilution factor provided to account for this.

(2) The relatively large Peclet number of geosphere layer 2 may cause instability in submodels relying on a numerical solution to the transport equations.

(3) Some participants considered the case specification to be ambiguous as concerns the area to be used for solubility calculations within the repository vault; different assumptions for vault area would affect the implied dilution in the geosphere of solubility-limited radionuclides.

2.4 Biosphere

The very simple biosphere model imposed in the case specification was used by all participants.

2.5 Parameter Distributions

All parameter values and distributions were specified, and were used by all of the participants with two exceptions:

(1) One participant (K) mistakenly did not sample from the sorption distributions provided for the stochastic analyses, but used instead the fixed values provided for deterministic case 3.

(2) Another participant (I) encountered difficulty in allowing for the absence of correlation between velocities in the two geosphere layers, because the code solves for groundwater flow prior to solving the transport equations.

3. PRESENTATION AND DISCUSSION OF RESULTS

3.1 Introduction

The Level 1a case specification formed the basis for a variety of potentially interesting analyses, and participants were encouraged to provide the Task Group with all available information on their studies, including any problems encountered. Because different modelling approaches could be applied in the Level La exercise, it is not possible to compare the performance of the codes against a "correct" answer. The intention throughout has been to understand to what extent different results can be attributed to different modelling approaches, and which assumptions are of primary significance to the results obtained.

Because the models and assumptions adopted by the participants were not identical, results from the three deterministic cases were closely examined. These three cases were constructed from consideration of the ranges of parameter values specified for the stochastic runs:

DETRUN1 "Pessimistic case"

The parameter value at the limit of the distribution giving rise to the fastest radionuclide transport and, where relevant, the highest dose, was systematically chosen.

DETRUN2 "Optimistic case"

The parameter value at the limit of the distribution giving rise to the slowest radionuclide transport and, where relevant, the lowest dose, was systematically chosen.

DETRUN3 "Central case"

Medians of the distributions specified for the stochastic runs were chosen.

Initially, various graphical analyses were used to compare the results, and hand calculations (e.g., of transport time) were used to check the consistency of results with the data provided in the case specification. The participants involved at this early stage were invited to use this comparative information to confirm or modify their results. The purpose of this first iteration was to eliminate, to the extent possible, bias due to data misinterpretation and encoding errors. Some participants submitted new sets of results and additional contributions were later received from other parties, who had not contributed during the first iteration. Participation in these two iterations is summarised in Table 1.1.

This Section of the report begins with a general overview and comparison of the deterministic and stochastic results obtained (Section 3.2). The subsequent nine Sections (3.3-3.11) provide a detailed presentation and discussion of the individual results. Times of peak dose and peak dose rates from the three deterministic runs are discussed in Section 3.3 and 3.4. Sections 3.5-3.9 focus on the importance of particular modelling approaches and interpretations of the specification, and their influence on the final results. Section 3.10 contains a discussion of the results from the stochastic runs, and in Section 3.11, an attempt is made to weigh variations arising from variability in the input data against those arising from the use of different modelling approaches.

It should be stressed that the lack of an exact solution is inherent to the Level 1a exercise. Consequently, agreement between sets of independently generated results only provides evidence - and not proof - that the respective codes are functioning correctly. Similarly, codes that produce results that differ significantly from those generated by other codes should not necessarily be considered as functioning incorrectly, particularly insofar as some codes had to be used outside their stated domain of application, in order to simulate the case.

3.2 General Overview of Results

The aim of this Section is to provide a description of the results in general terms, prior to proceeding to a more detailed analysis. Principal component analysis (PCA) was among the tools used to analyse the results. Explained in detail in the Level 0 report [1], PCA aids in visualising the general disposition of the data, and in identifying those participants whose results on a global level tend to cluster, and those participants whose results on a global level tend to be outliers.

Figures 3.1a (first and second components) and 3.1b (first and third components) show PCA projections that include most results for all participants except G. These two figures illustrate a general trend in the data, which is confirmed by the more detailed analysis presented in Sections 3.3-3.10:

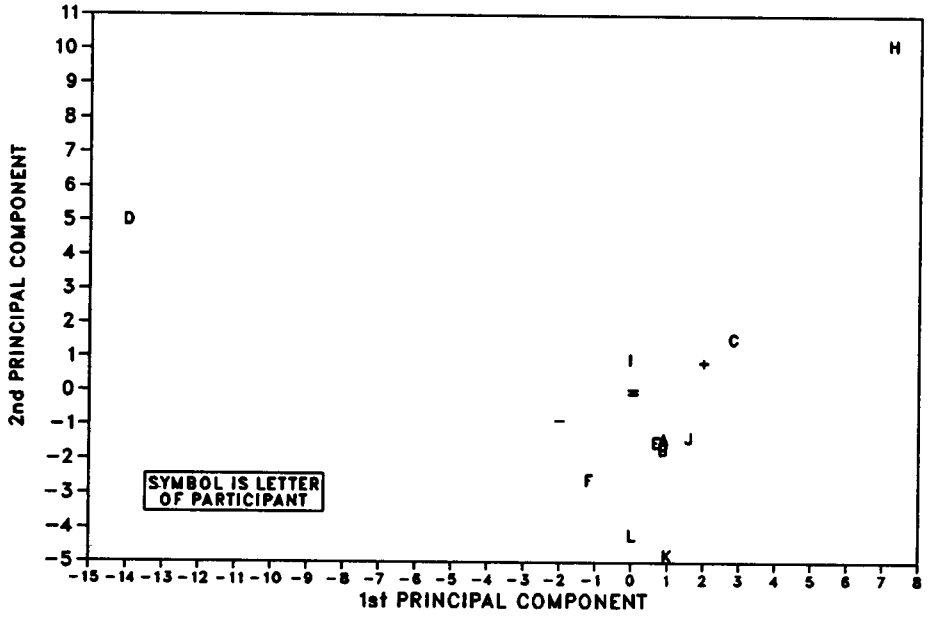
- the results from participants D and H on a global level are considerably different from those of the other participants;
- a relatively tight cluster is formed by participants A, B, E, and J; and
- the global results from participant F are relatively close to those of A, B, E and J, whereas those from participants K and I exhibit a relatively large spread on the third axis (Fig. 3.1b).

As shown in Section 2, participants A, B, C, E, and J were able to conform exactly to the proposed specification, although their numerical methods, particularly with regard to the repository vault, were different. With the exception of participant C, these participants generated a relatively

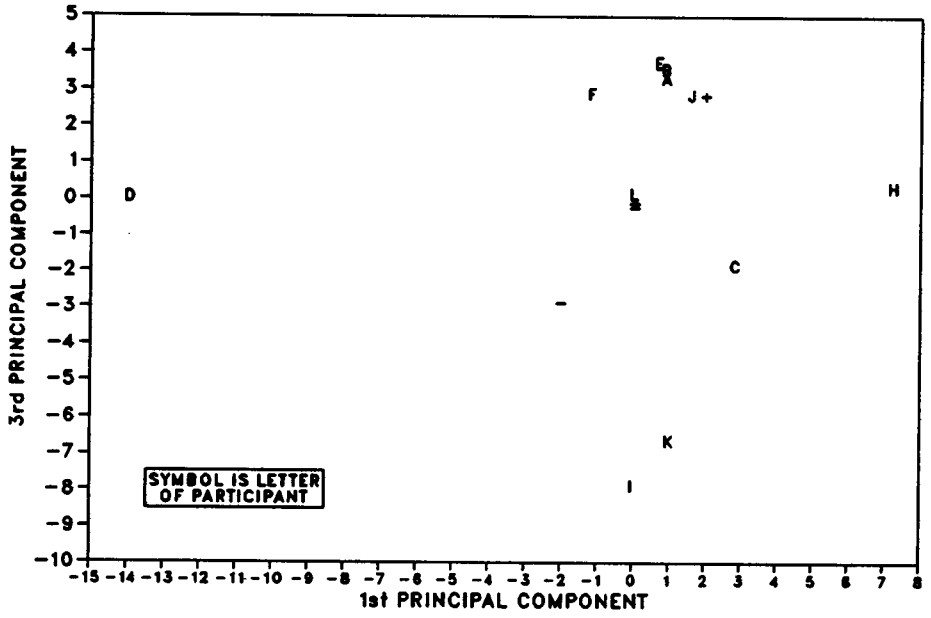
Fig. 3.1: Principal component analysis of all possible results.

The three fictitious points '=', '+' and '−' represent the mean (0,0), mean + 1 s.d. and mean − 1 s.d. and were zero-weighted in the analysis. Participant G was excluded, and the other participants' results were each given equal weight.

(a) 2nd vs. 1st principal component



(b) 3rd vs. 1st principal component



tight cluster for all responses to the questionnaire, as suggested by PCA (Fig. 3.1). The results for participant C, however, are those from the first iteration of participant J; this earlier iteration was retained in order to illustrate the role of different interpretations of the case specification (see detail in Annex B and Section 3.8). The clustering of results reduces the likelihood of data misinterpretation or encoding errors for participants A, B, E, and J.

3.2.1 Deterministic Results

An overview of the deterministic results is obtained by considering peak dose rates and times of peak for various radionuclides. For any single participant it is expected, based on the case specification, that the time of peak dose would increase systematically from DETRUN1 to DETRUN3 to DETRUN2 (whereas the peak dose itself would decrease systematically). Considering just the I-129 results for the three deterministic cases, it can be seen that this observation is valid (Fig. 3.2). Moreover, for the total set of 11 participants providing results, the minimum peak time (of the 11) for DETRUN3 (the central case) is greater than the maximum peak time (of the 11) for DETRUN1, and the maximum for DETRUN3 is less than the minumum for DETRUN2. Insofar as iodine is, however, a nonsorbed species with a high solubility limit, these results do not incorporate all of the processes of interest.

The fast transport case (DETRUN1) shows particularly good agreement between participants. Agreement is less good for the slowest case (DETRUN2). There is a direct correlation between this observation and differences in the maximum release rates from the vault provided by the participants (Fig. 3.3). The DETRUN1 release curves from the vault occur almost instantaneously on a million year time-scale. In contrast, results from the slower cases (DETRUN2 and DETRUN3) show significant differences in estimated releases from the repository vault, differences which are propagated through to the dose estimates. Results from a larger variety of intermediate cases would have identified the reasons for these differences, but such results were not requested of participants.

These observations are equally relevant for the other nuclides studied For example, the U-238 peak dose rates and times of peak from the various participants form a small cluster for DETRUN1 (Fig. 3.4). DETRUN3 is uninformative because the dose-vs-time curves reach a plateau, with the time of peak being poorly defined. Even participants A, B, E, and J differ as to the time of peak, although their estimates of dose rates do agree. DETRUN2 does not give rise to appreciable dose rates from U-238 over the period studied. The corresponding release rates versus time are shown in Fig. 3.5.

In summary, the deterministic results are, in general, grouped in a relatively small cluster compared with the uncertainties normally observed in stochastic assessments of deep disposal sites.

3.2.2 Stochastic Results

As mentioned in Section 2.5, not all participants conformed strictly to the case specification for sampled parameters. The different types of model sometimes imposed a different use of the parameters and alternative interpretations of the sampling required. Nonetheless, for the Level 1a exercise, notwithstanding some differences in interpretation, most

Fig. 3.2: Peak dose rates from I–129 versus times of peak for the three deterministic runs.

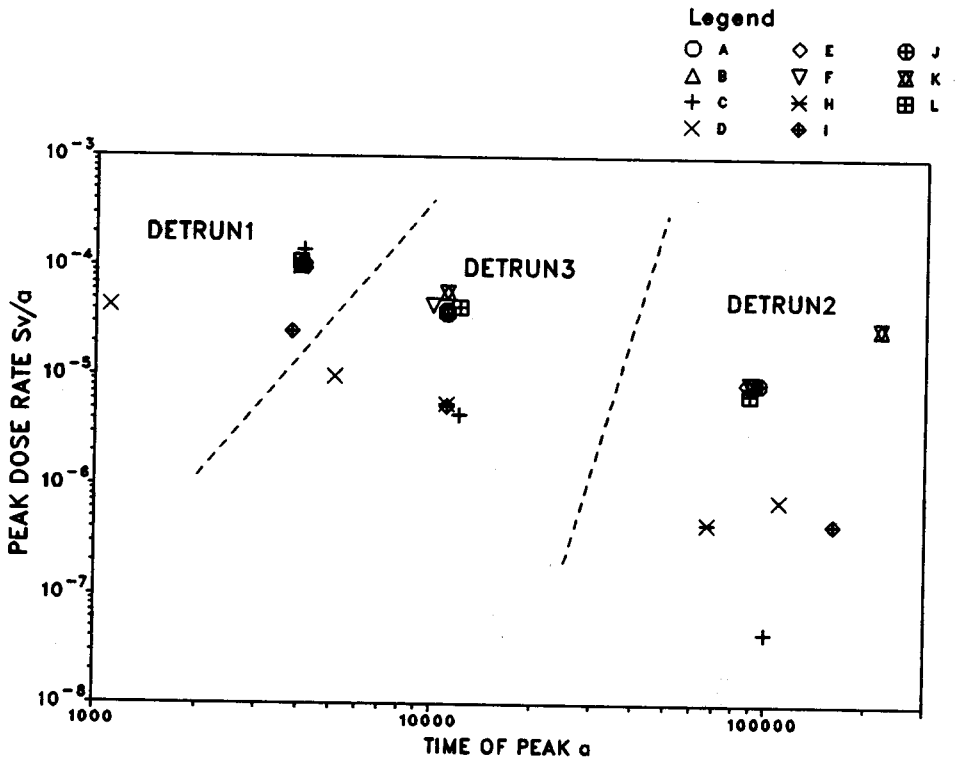


Fig. 3.3: Release rates from the repository vault at selected times for I–129, for each of the deterministic runs.

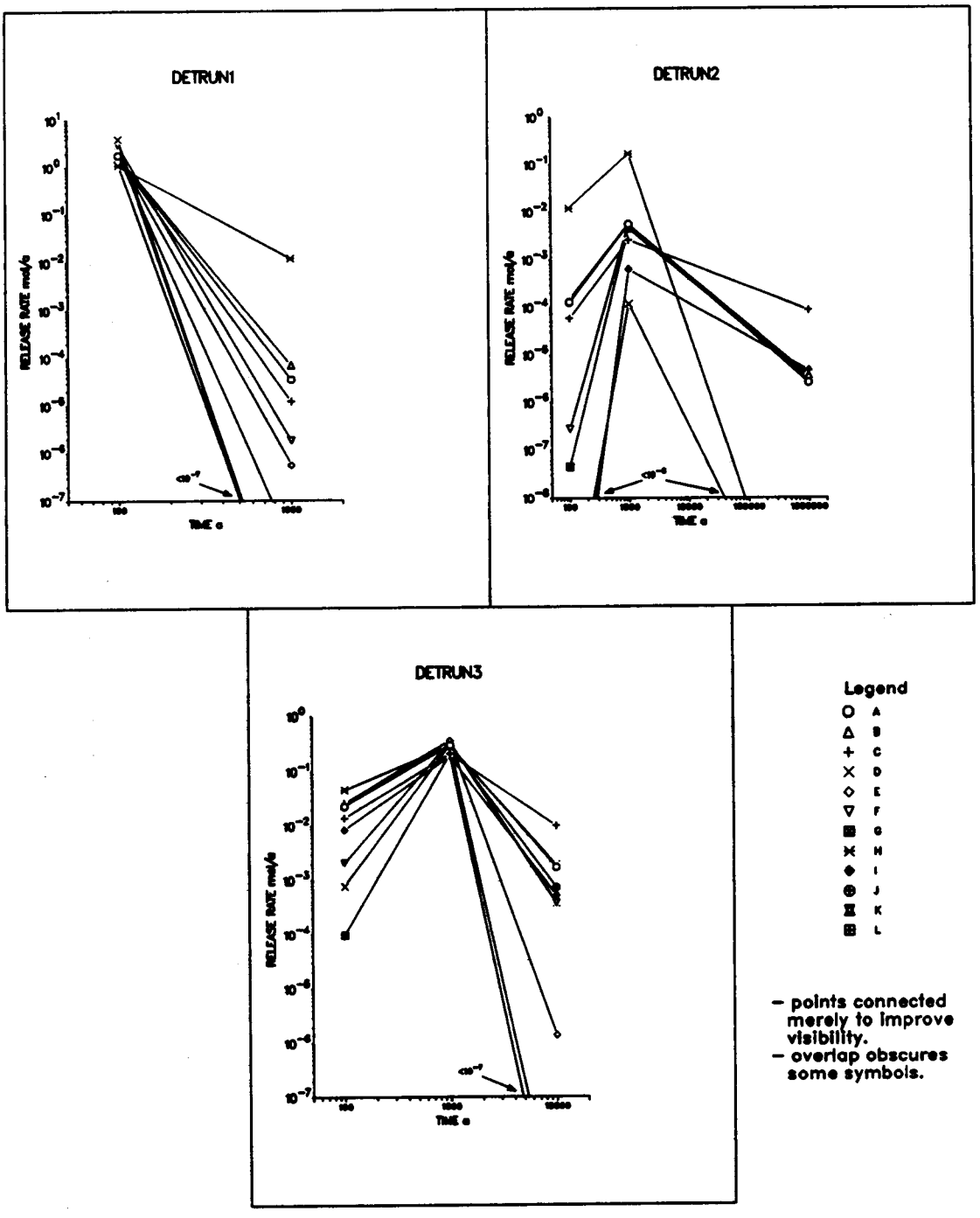


Fig. 3.4: Peak dose rates from U–238 versus times of peak for DETRUN1 and DETRUN3.

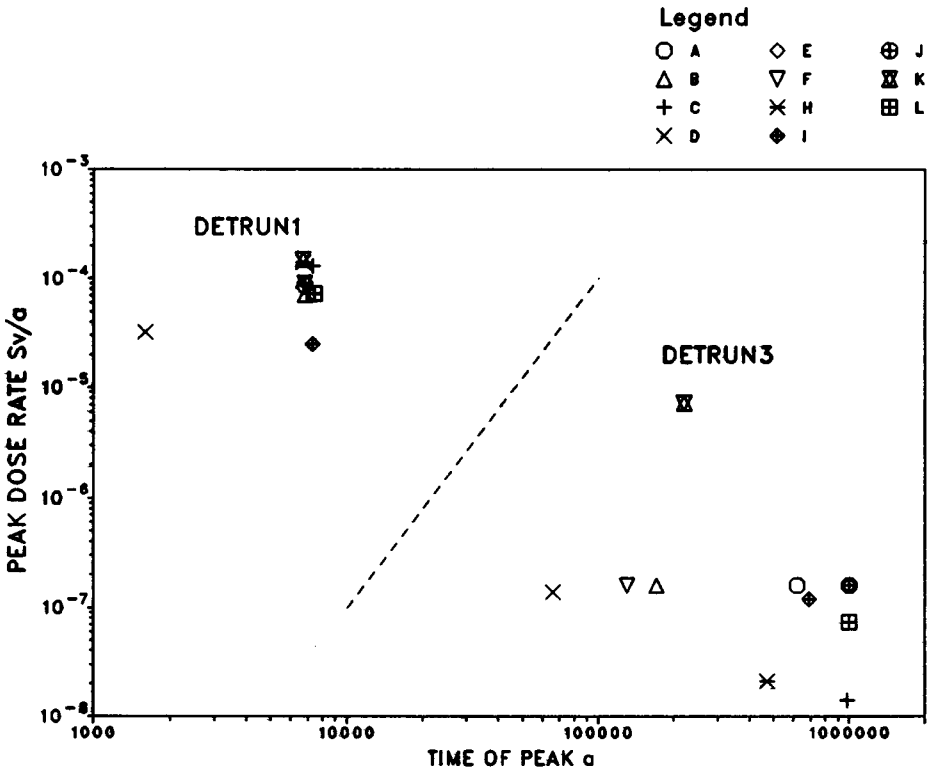
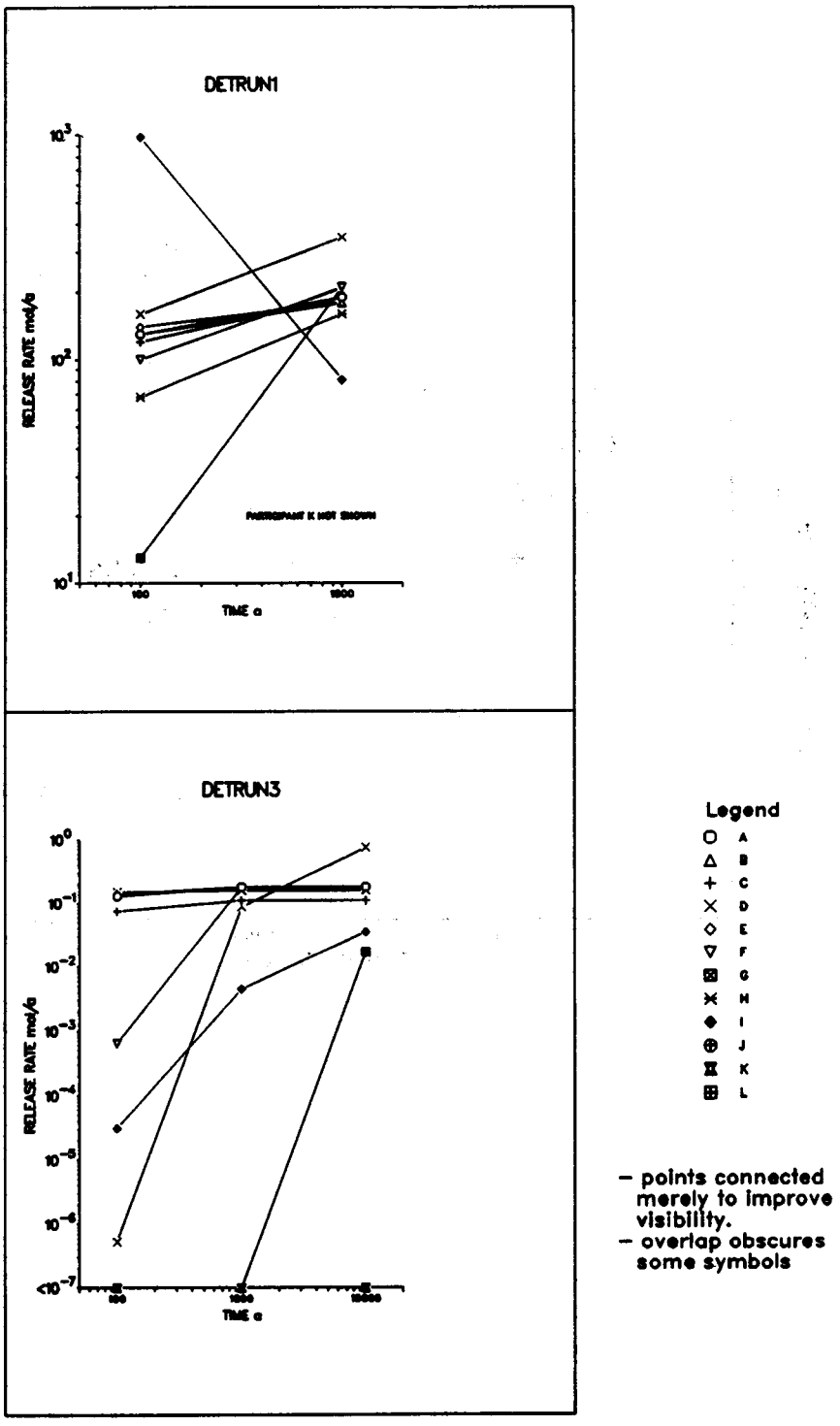


Fig. 3.5: Release rates from the repository vault at selected times for U–238, for DETRUN1 and DETRUN3.



parameter value distributions were sampled identically by most participants. Figure 3.6 shows the stochastic results obtained by the eleven participants. Participants were asked to provide confidence limits on the expectation values of dose, in order to represent ranges of uncertainty attributable to the sampling approaches adopted.

As expected, the general disposition of expectation values of dose rates at 10,000 years resembles the general disposition of peak dose rates from I-129 calculated in DETRUN3 - the "central case". At other times, when dose rates are smaller, there is generally better agreement between the results from the various participants than that at 10,000 years.

It should be noted that the constraints imposed by the Level 1a case specification may well have artificially limited the influence of model uncertainty in this exercise. The results obtained indicate that it is appropriate to proceed to a more complex exercise, in which a more general specification of a particular disposal concept at a specific site is provided to participants.

A detailed comparison of results is provided in Sections 3.3-3.11 of the report.

3.3 Times of Peak Dose

Question C3 of the questionnaire asked participants to give peak dose rates and times of peak for all three deterministic runs for five selected nuclides: Tc-99, I-129, Np-237, U-238, and U-234. This question has been answered in 11 of the 12 contributions. Participant G did not provide an answer because the code used (STRAW) does not include a geosphere model, and is designed only for the calculation of nuclide releases from a repository vault.

For this exercise, time of peak dose can be estimated from travel times through the two geosphere layers and release times from the vault and waste packages. Whereas calculation of the latter is complicated, geosphere travel times can be derived from the input data in a straightforward way. Advective travel time T of element e through layer i is obtained as

$$T_i(e) = [R_{fi}(e)]\ [LPATH_i]\ [PORL_i / VDARCYL_i], \qquad (3.1)$$

with

$$R_{fi}(e) = 1 + [\rho_i]\ [1 - \varepsilon_i]\ [k_{di}(e) / \varepsilon_i]. \qquad (3.2)$$

Input values for rock density ρ_i and total porosity ε_i of layer i, as well as element- and layer-specific k_d values, are given in Tables 1 and 4 of the case specification (see Annex A). The meaning and values of the three random variables in Eqn. (3.1) are also found in these Tables. The resulting retardation factors $R_{fi}(e)$ and travel times are given in Table 3.1. The calculated times of peak dose can be less than these estimated travel times

Fig. 3.6: Stochastic results for the PSACOIN level 1a exercise, showing
(a) mean dose rates at six specified times
(b) mean dose rate and 95% Chebychev confidence bounds
at each of the six times (six plots).

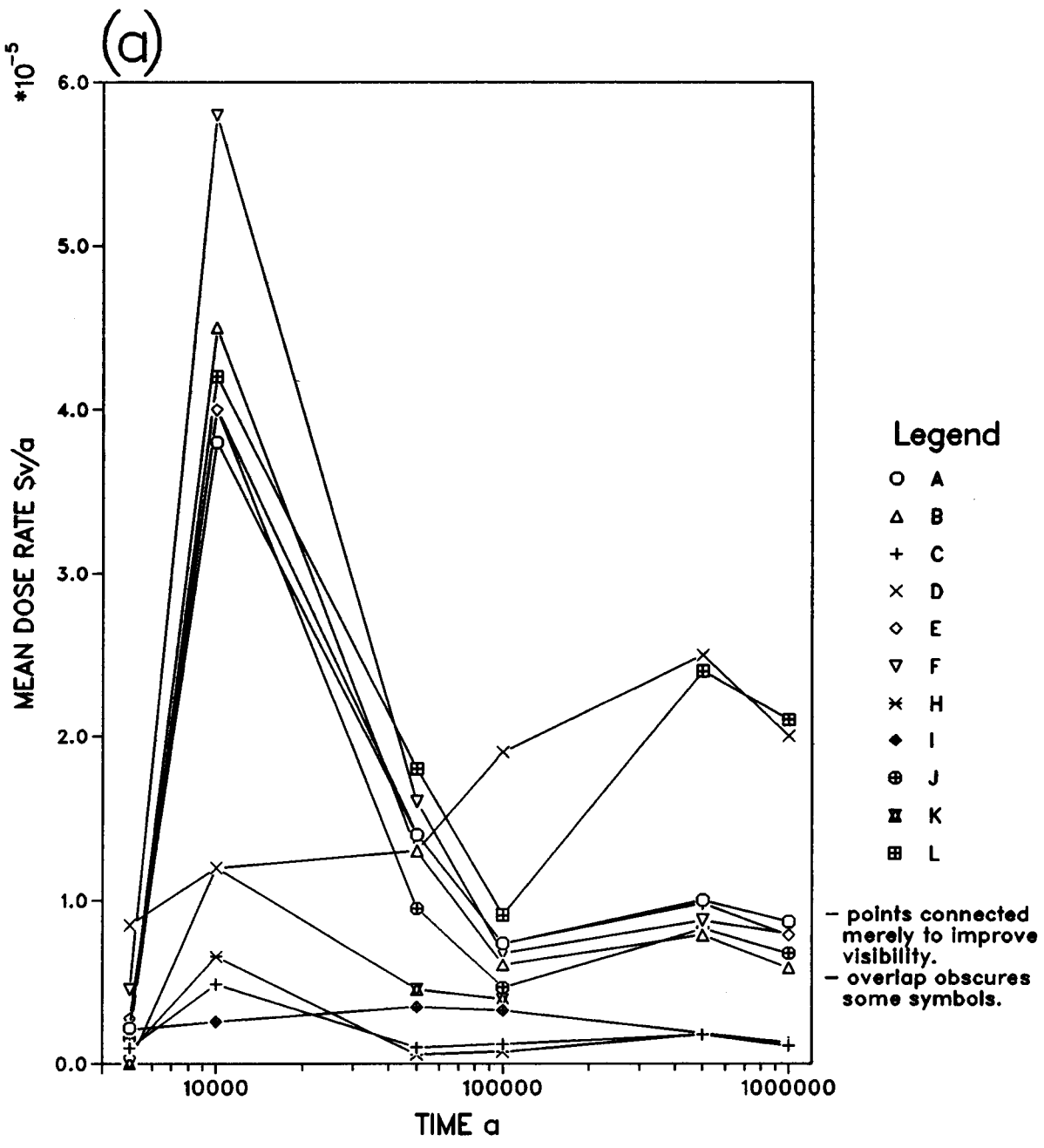


Fig. 3.6: (Contd.)

(b)

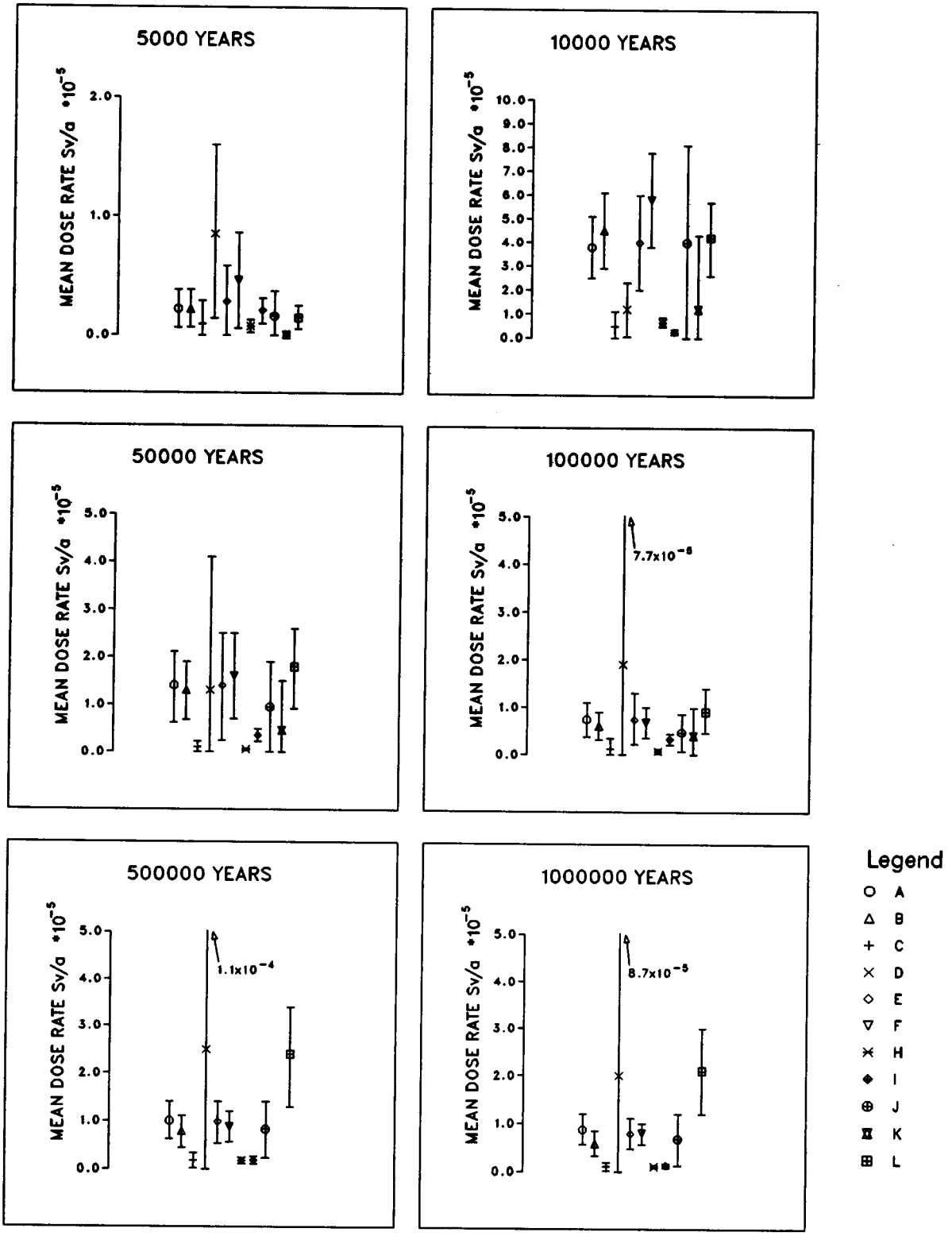


Table 3.1: Estimates of element-specific radionuclide travel times through the geosphere for the three deterministic runs.

RUN	ELEMENT	RETARDATION FACTORS LAYER 1	RETARDATION FACTORS LAYER 2	TRAVEL TIME LAYER 1 (YEARS)	TRAVEL TIME LAYER 2 (YEARS)	GEOSPHERE TRAVEL TIME (YEARS)
DETRUN1	Tc	1.24	1.19	558	4046	4604
	I	1.0	1.0	450	3400	3850
	Np	5.83	4.75	2624	16150	18774
	U	3.41	1.38	1535	4692	6227
DETRUN2	Tc	25.1	19.8	276100	$> 10^6$	$> 10^6$
	I	1.0	1.0	11000	57500	68500
	Np	484	376	$> 10^6$	$> 10^6$	$> 10^6$
	U	242	38.5	$> 10^6$	$> 10^6$	$> 10^6$
DETRUN3	Tc	3.41	2.87	4651	23425	28076
	I	1.0	1.0	1364	8162	9526
	Np	49.3	38.5	67245	314237	381482
	U	25.1	4.75	34236	38770	73006

owing to dispersion in the geosphere; peak doses can also occur later since the time for release from the vault has been neglected. It will be considered in the subsequent discussion of participants' results whether either of these opposite effects can plausibly account for individual differences.

Table 3.2 shows the estimated travel times together with participants' results for time of peak dose and some indications of deviations, for each nuclide considered and for each of the three deterministic runs. Selected examples from this Table are illustrated in Fig. 3.7. Most estimates for time of peak dose are within about 10% of the mean value. An exception is recognised for U-238 in DETRUN3, where the results spread over one order of magnitude. In DETRUN3, however, the U-238 dose rate is almost constant over the corresponding time period owing to a constant U-238 release from the vault, which in turn is controlled by the solubility limit. Although solubility limits are element-specific, participants' results also show that U-234 does not follow this trend because of its higher decay rate.

Results from participant D show a systematic deviation: computed times of peak are significantly (usually by a factor 2 to 4) earlier than those from any other participant. Indeed, the times of peak calculated by this participant are significantly earlier than the estimates given in Table 3.2. For I-129, the calculated time of peak dose is much earlier than the groundwater travel time. Given the Level 1a data set, this discrepancy cannot be due to dispersion in the geosphere.

Further deviations are noticed in some results of participants K, L, and I. For example, for I-129 in DETRUN2 or Np-237 and U-234 in DETRUN3, these participants have calculated later times of peak (see Table 3.2). Note that these cases all involve long transit times with late peak arrival. For participant L, this deviation is traced back to a different approach to vault modelling in Section 3.8. For I-129 in DETRUN1, participant I obtained a time of peak that is slightly smaller than that from the bulk of results, and this discrepancy again cannot be attributed to dispersion.

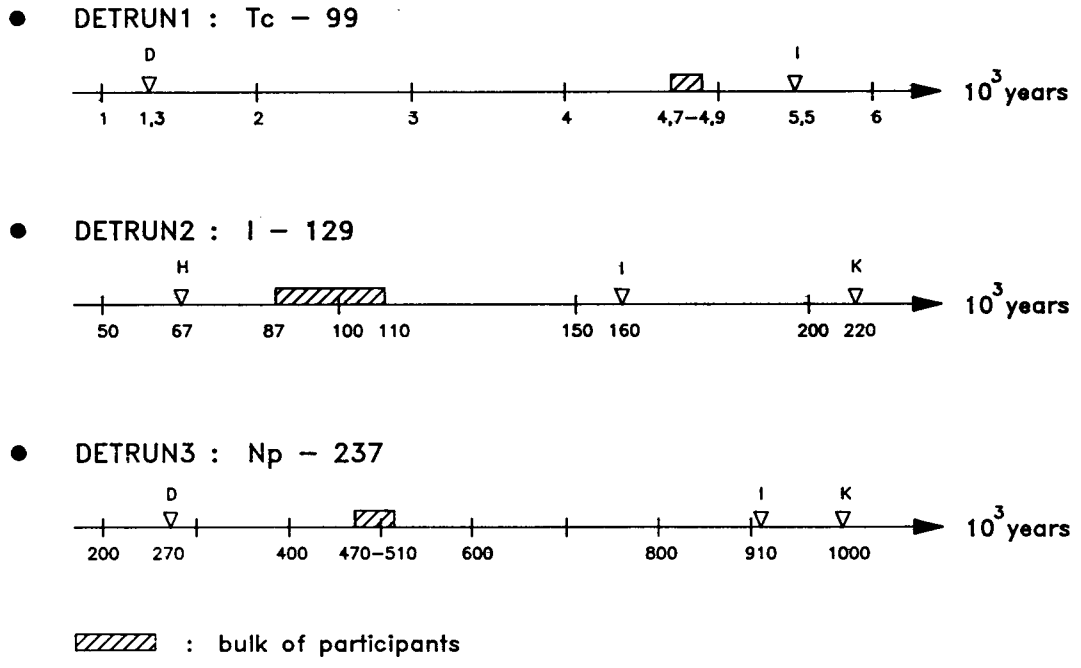
An interesting deviation is obtained by participant H for I-129 in DETRUN2. The calculated time of peak is some 30% earlier than the results of other participants, and almost identical with the estimated geosphere travel time given in Table 3.2. A possible explanation is that diffusive transport out of the vault, which has been modelled only by H, dominates in this run. A detailed discussion of how a different approach to vault modelling by participant H affects calculated times of peak dose is included in Section 3.5.

In summary, it should be stressed that the bulk of participants' calculated times of peak dose are in excellent agreement. One participant obtained significantly smaller times of peak dose, which are obviously erroneous. In a few cases with late arrival times, some participants calculated times of peak dose as much as a factor of 3 larger than the bulk. Some of these differences can be traced back to different approaches to vault modelling (see Section 3.7). In DETRUN2, participant H obtained smaller times of peak than the other participants. This will be further discussed in Section 3.5.

Table 3.2: Overview of participants' calculated times of peak dose rate for the three deterministic runs.

RUN	NUCLIDE	ESTIMATE (YEARS)	RANGE WITH BULK OF PART. (YEARS)	DEVIATIONS (PARTICIPANT: YEARS)
DETRUN1	Tc- 99	4604	4700 - 4900	D: 1300 / I: 5500
	I -129	3850	4000 - 4100	D: 1100 / I: 3800
	Np-237	18774	20000 - 24000	D: 4300
	U -238	6227	6700 - 7400	D: 1600
	U -234	6227	6700 - 7300	D: 1600
DETRUN2	Tc- 99	> 10^6	> 10^6	D: 510000
	I -129	68500	87000 - 110000	K: 220000 / I: 160000 / H: 67000
	Np-237	> 10^6	> 10^6	
	U -238	> 10^6	> 10^6	
	U -234	> 10^6	> 10^6	
DETRUN3	Tc- 99	28076	29000 - 36000	D: 9300
	I -129	9526	10000 - 12000	D: 5100
	Np-237	381482	470000 - 510000	K: 1000000 / I: 910000 / D: 270000
	U -238	73006	130000 - 1000000	D: 66000
	U -234	73006	100000 - 130000	L: 400000 / K: 220000 / I: 180000 / D: 51000

Fig. 3.7: Selected examples for the three deterministic runs showing representative deviations for calculated times of peak dose.



3.4 Peak Dose Rates

Analysis of deviations in peak dose rates is more complicated than for times of peak, where estimated travel times were of help. Observations (rather than explanations) are given for the three deterministic runs. As for the times of peak, all participants except G calculated peak dose rates.

An overview of calculated peak dose rates for each nuclide and for each of the three deterministic runs is given in Table 3.3, and selected examples from this Table are illustrated in Fig. 3.8. As for the times of peak dose, there is a range of values containing the bulk of participants' results. This range is typically much smaller than one order of magnitude, with the only exception being for Np-237 in DETRUN3, where the range is slightly larger. Considering the degree of freedom allowed in modelling the Level 1a case, this general agreement is encouraging.

In DETRUN1, a systematic deviation of peak doses by participant I is evident. Calculated peak doses are typically a factor of 4 to 5 smaller than the mean value of other participants' results. This is the more striking since all other results are quite close to each other, apart for participant D, whose results have been identified as erroneous in Section 3.3. There is no clear relationship between participant I's lower peak dose rates and his release rates from the vault. Whereas release rates are relatively high for U-238, they show a drastic decrease between 100 and 1000 years for I-129, but almost no decrease for Tc-99 in the same period. It appears more likely that participant I's modelling of geosphere transport plays a role: this modelling includes an implicit dilution occurring within the layers. The dilution factor given in the case specification therefore had to be corrected to account for already diluted concentrations arriving at the geosphere/biosphere interface.

The tendency of participant I to underestimate peak dose values is again evident in DETRUN2 and DETRUN3 for Tc-99 and I-129, although his results do lie within the range of the other paticipants' results for the other nuclides in these two runs. Other deviations in these runs include results from participants C and H, who also calculated lower peak dose rates. In particular, participant C obtained a peak dose value for I-129 in DETRUN2 more than two orders of magnitude lower than that of the bulk of participants.

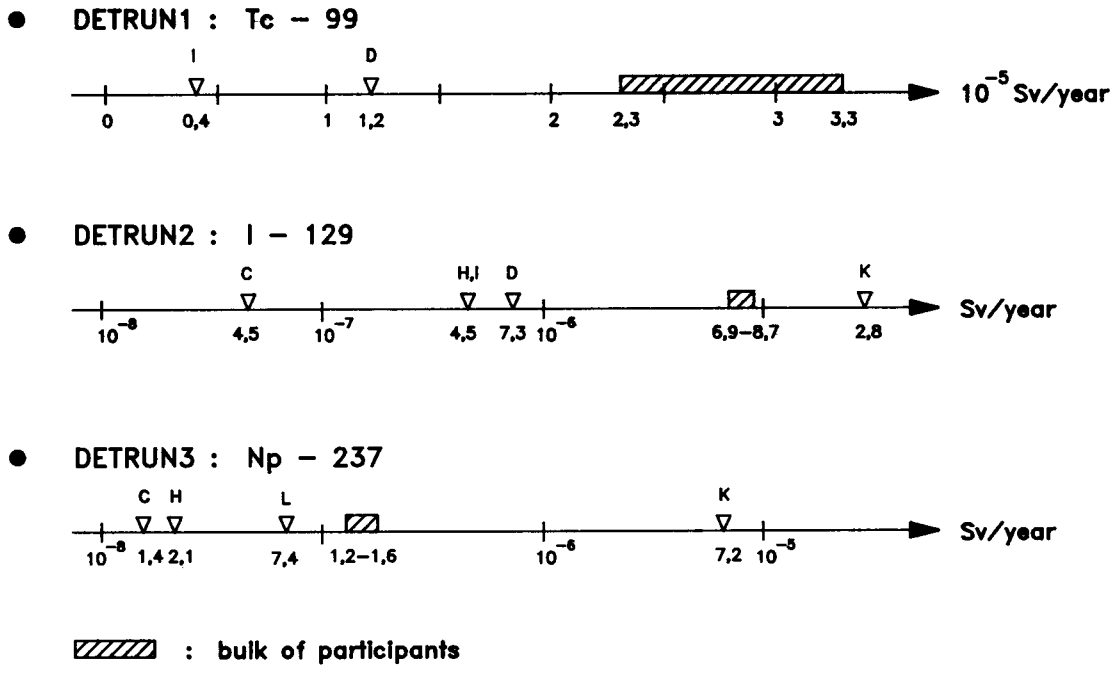
Participant C's lower dose rates can be traced back to different vault modelling. His release rates for I-129 in DETRUN2 and DETRUN3 are lower for earlier times (100 and 1000 years), whereas they are the largest at later times (10,000 and 1,000,000 years). A similar effect is observed for Tc-99, although it is blurred in DETRUN2 where Tc exceeds its solubility limit. It can be concluded that the time history of the release rate is extended over a longer period, thereby resulting in lower peak release rates. The differences in participant C's vault modelling leading to these differences in release rates are discussed in further detail in Section 3.7.

In contrast to other deviations, participant K's calculated peak doses are higher than average, especially for the two Uranium nuclides in DETRUN3, where the deviation is up to two orders of magnitude. An attempt has been made to trace back these higher Uranium peak dose rates to release rates from

Table 3.3: Overview of participants' calculated peak dose rates for the three deterministic runs.

RUN	NUCLIDE	RANGE WITH BULK OF PART. (SV/YEARS)	DEVIATIONS (PARTICIPANT: SV/YEARS)
DETRUN1	Tc- 99	2.3E-5 - 3.3E-5	I : 4.0E-6 / D : 1.2E-5
	I -129	9.8E-5 - 1.4E-4	I : 2.5E-5 / D : 4.3E-5
	Np-237	3.5E-4 - 8.1E-4	I : 1.0E-4 / D : 1.1E-4
	U -238	7.1E-5 - 1.5E-4	I : 2.5E-5 / D : 3.2E-5
	U -234	1.5E-4 - 3.0E-4	I : 5.2E-5 / D : 6.7E-5
DETRUN2	Tc- 99	1.0E-11 - 5.5E-11	K : 0. / C : 1.3E-13 / D: 2.8E-9 / I: 1.9E-12
	I -129	6.9E-6 - 8.7E-6	C : 4.5E-8 / H,I: 4.5E-7 / D: 7.3E-7 / K: 2.8E-5
	Np-237	0.	I : 1.4E-15
	U -238	0.	D : 1.9E-12 / I : 2.3E-15
	U -234	0.	D : 2.1E-12 / I : 4.2E-14
DETRUN3	Tc- 99	3.6E-6 - 5.2E-6	C,I: 4.7E-7 / H : 5.7E-7 / D: 1.5E-6
	I -129	3.7E-5 - 5.8E-5	C : 4.4E-6 / I : 5.3E-6 / H: 5.6E-6 / D: 9.8E-6
	Np-237	3.8E-7 - 5.5E-6	
	U -238	1.2E-7 - 1.6E-7	K : 7.2E-6 / C : 1.4E-8 / H: 2.1E-8 / L: 7.4E-8
	U -234	2.2E-7 - 3.0E-7	K : 1.2E-5 / H : 3.8E-8 / L: 2.0E-6

Fig. 3.8: Selected examples for the three deterministic runs showing representative deviations for calculated peak dose rates.



the vault. However, participant K has calculated zero or extraordinarily small release rates at all time points for all nuclides and almost all runs and, therefore, an element-specific effect to account for higher Uranium peak dose rates could not be detected.

A more global look at the results obtained for both peak dose rates and times of peak has been presented previously in Figs. 3.2 and 3.4 for I-129 and U-238, respectively. The different runs do not overlap and can easily be distinguished. DETRUN2 only appears for I-129 since the peak is not reached for U-238. It can be observed that the spread of results for DETRUN3 is larger than for DETRUN1. Also, for I-129, it appears that DETRUN2 presents a greater spread between the participants than DETRUN3.

These observations could have been predicted for DETRUN1, being a case of fast release combined with fast transport. The release curves on a million-year scale effectively present a Dirac impulse shape, and any differences would not be expected to be propagated through the geosphere because of dispersion. In contrast, in DETRUN3, for which releases are relatively slow, differences between the participants' results are, as expected, propagated through to the dose estimates. The I-129 DETRUN2 results confirm these observations.

In summary, the bulk of participants show good agreement in peak dose rates, although the range of results is somewhat broader than for the times of peak. Lower peak dose rates obtained by some participants are partly due to different vault modelling (participant C) or, presumably, to different modelling of dilution (participant I), or to a combination of both (participant H, see Section 3.5). Higher values for peak dose rates obtained by participant K could not be further explained. The spread in both peak dose rates and times of peak increases from DETRUN1 through DETRUN3 to DETRUN2.

3.5 Modelling of Diffusion from the Repository

In writing the Level 1a case specification, the choice of modelling approaches was left to the participants as far as possible. Accordingly, though advective transport of radionuclides from the vault had been suggested in the specification, other transport processes were not explicitly excluded. In the absence of input data for diffusive transport, most of the participants decided to model advective transport only. Participant L artificially suppressed diffusion in his model in order to follow this general approach. Participant H, however, chose to model diffusion of radionuclides through the repository walls, in addition to advective transport.

In general, water passes relatively slowly through the empty voids of the vault, with most water bypassing the vault altogether. The relative importance of radionuclide diffusion increases with lower water velocity within the vault, i.e., in terms of the specification, with lower values of FDARCYVLT. Participant H modelled diffusive transport only for values of FDARCYVLT less than unity, i.e., as long as water velocity within the vault was less than that outside the vault. Furthermore, diffusion was only modelled through the vault's walls in directions orthogonal to the direction of water flow.

There is no diffusive transport in DETRUN1, and differences there must have other causes. Participant H's release rates in DETRUN1 are generally at the lower end of the bulk range, whereas they are particularly high for Tc-99 and I-129 at 1000 years. This will be further discussed in Section 3.8. A major effect of the additional modelling of diffusion is expected in DETRUN2 and, to a lesser extent, in DETRUN3. According to interim results obtained by participant H (see Annex B), diffusive transport is the dominant process in DETRUN2, and is of the same importance as advective transport in DETRUN3.

These predictions are verified through comparison with other participants' results. Throughout DETRUN2, participant H obtained the highest release rates from the vault for all nuclides and all time points, until the inventory is exhausted, as can be observed for Tc-99 and I-129 at 1,000,000 years. The difference with other participants' release rates is typically at least one to two orders of magnitude.

The effect of modelling diffusion can still be observed in a comparison of release rates in DETRUN3. In particular, at 100 years after repository closure, release rates of Tc-99, I-129, and Np-237 obtained by participant H are almost exactly twice those obtained by several other participants, including A, B, E, and J. This confirms the approximately equal importance of diffusive and advective transport in DETRUN3.

This relationship between participant H's release rates and those from other participants is not observed for the estimates of total dose rates at selected time points. Here, an almost reverse relationship prevails: while participant H's total dose rates are amongst the highest calculated in DETRUN1, they are relatively small in DETRUN3 and particularly low in DETRUN2. Hence, the demonstrated effect of diffusion on release rates is superimposed by another stronger effect when it comes to calculation of doses. Dilution plays a decisive role in this respect, and this will be explained in Section 3.8.

Another peculiarity of participant H's results in DETRUN2 is the early arrival time of peak dose for I-129. This has already been mentioned in Section 3.3 and the effect can only be observed for I-129, since times of peak dose for all other selected nuclides are beyond the cut-off time of 1 million years specified for the exercise. Participant H's smaller time of peak dose can be traced back to a different time history of I-129 release rate, owing to diffusive transport out of the vault. Figure 3.9 shows time histories of I-129 release rate in DETRUN2 as calculated by participants H and A, the latter taken as representative of the participants not considering diffusive release. Both curves in Fig. 3.9 have their maximum around 1000 years after repository closure. The maximum release rate calculated by participant H is significantly higher, owing to diffusive release. The I-129 inventory in the vault is thereby exhausted sooner, leading to a relatively rapid decrease of release rates. Because the time of maximum release rate is small compared to the geosphere travel time of some 68,000 years, a time of peak dose of this order of magnitude, as calculated by participant H, is plausible. In contrast, the release rate calculated by other participants has a lower maximum level, but is almost constant over a period of time from 1000 to 100,000 years, thereby leading to a later arrival time of peak dose.

Fig. 3.9: Time histories of I-129 release rates from vault in DETRUN2 for participants A (1) and H (2).

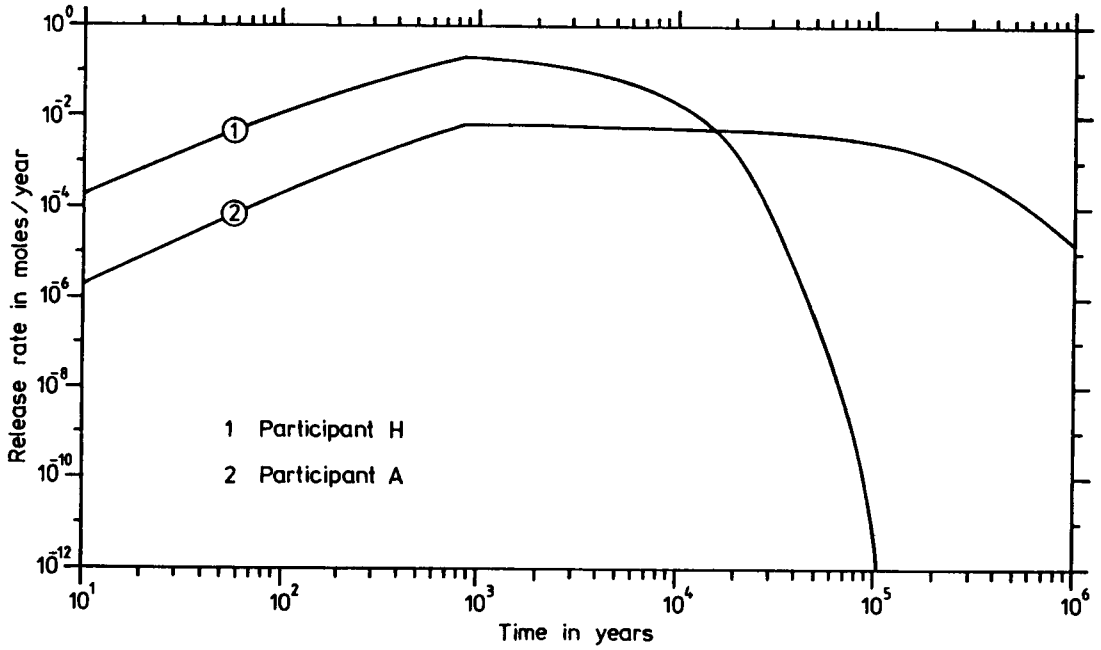
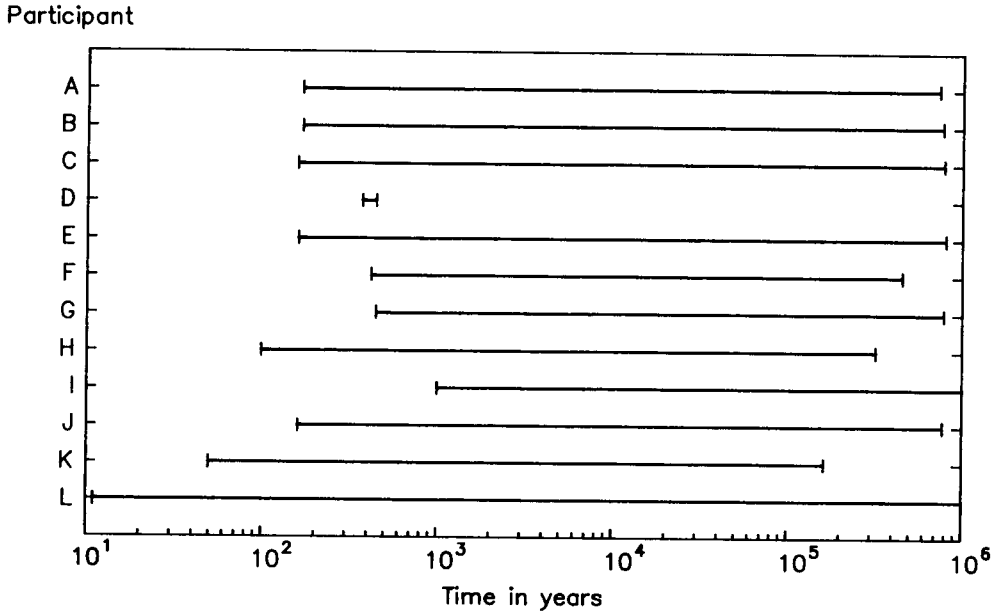


Fig. 3.10: Periods exceeding solubility limit of Tc in DETRUN2 for each participant.



Summarising the importance of modelling radionuclide diffusion from the vault for the Level 1a exercise, it has been shown that there are a large variety of input parameter values for which diffusion contributed (significantly) to the total release out of the vault. Further influence on calculated doses is superimposed by other modelling differences, particularly as concerns the modelling of dilution. It has been shown, however, that modelling diffusion out of the vault can lead to 30-40% earlier times of peak dose for this particular exercise.

3.6 Modelling of Solubility Limits

The Level 1a case specification includes precipitation of radionuclides as a process to be modelled within the repository vault. According to the specification, precipitation occurs whenever element-specific solubility limits are exceeded. There are several isotopes of the same elements among the 13 radionuclides selected for the exercise. Compliance with the specification therefore requires a vault model which includes multiple-isotope precipitation.

The vault models of some participating codes could not account for this process, or could not simulate precipitation at all. Nevertheless, all participants gave answers to question C2 of the questionnaire, which asked for the times between which selected elements exceed their respective solubility limits. In the absence of an appropriate model to answer this question, participants resorted to various improvisations.

Because a vault model is not part of participant K's code (NEFTRAN), solubility limits were not used except for comparison with calculated concentrations, and then they were compared with the highest concentrations occurring within the vault, but outside the waste itself. The resulting periods typically start and end relatively early. In contrast to other participants, participant K obtained a period of 130 to 1400 years when Np-237 exceeds its solubility limit in DETRUN3. In addition, it is noteworthy that in this run participant K obtained a period of 130 to 1900 years when the Uranium solubility limit is exceeded in the vault, whereas at 1000 years, a Uranium release rate from the vault of zero was calculated.

Within the code used by participant I (VANDAL), solubility limits only apply to releases from waste packages. The argument for using such a model is that the highest concentrations are found within the waste packages, so that solubility limits should be most effective there. In comparison to the results of other participants, participant I's results do not show a clear tendency; for example, whereas the period of exceeding solubility limits starts relatively late for Tc-99, this period starts relatively early for Np-237. The period for U-238 is not detected in DETRUN1, and starts significantly later than that calculated by other participants in DETRUN2 and DETRUN3. It is particularly difficult to understand how a start time of 100,000 years can be obtained for the period for U-238 in DETRUN2, when release from the waste should, according to the case specification, have ended by 1000 years after repository closure.

The vault model used by participant L (SYVAC3) includes precipitation, but the simultaneous presence of different isotopes of the same element is not taken into account. Instead, the given value for the solubility limit for an element is used for each isotope in turn. With this approach, the calculated

periods of exceeding solubility limits should be generally shorter, but the opposite is the case. This is presumably due to the flow from the vault being smaller for participant L than for other participants (see Section 3.7), thereby leading to higher concentrations and, hence, longer periods of exceeding solubility limits, compared to other participants.

The code of participant G (STRAW) can account for multiple-isotope precipitation; it cannot, however, model the spread of the canister failure times and matrix degradation. An instantaneous radionuclide release from the waste packages was therefore assumed to take place at the mean of the maximum container lifetime (TDRUM) and matrix degradation time (TMATRIX). The same time was indicated as the beginning of exceeding solubility limits in question C2. This apart, participant G's results are comparable with a group of similar results obtained by participants A, B, C, E, and J.

Participant F used the same conceptual model as participant G, but the mathematical treatment was simplified. Question C2 could, therefore, only be answered approximately and, indeed, only the period during which the concentration exceeds half the solubility limits is reported. This provides the probable explanation of participant F's calculation of a period of 300 to 2100 years during which Tc exceeds its solubility limit in DETRUN3, and a significantly later end of the respective period for U-238 in DETRUN1. Against this trend, a relatively early end is calculated for Tc in DETRUN2.

Participant H obtained relatively early starting times for the periods of exceeding solubility limits, which can be explained by his modelling approach for the vault: the pore volume available for mobilised radionuclides increases with time as the number of failed containers increases. In contrast, many other participants assumed that the pore volume remained constant with time, and used the total pore volume of the waste packages from the very beginning. Hence, during the period of container failure, the available pore volume was considerably smaller in participant H's modelling and, therefore, solubility limits were exceeded earlier.

Participant D's results appear anomalous throughout, both for the elements and runs, which is most likely due to his approach to repository modelling (see Section 3.7).

In summary, the spread in the calculated periods of exceeding solubility limits is considerable (see Fig. 3.10). Differences in release rates out of the vault cannot, however, be related to the different approaches used to model radionuclide precipitation. In the context of the Level 1a exercise, therefore, it can be concluded that differences in modelling solubility limits are of minor importance.

3.7 Modelling Differences in the Repository

The Level 1a intercomparison had amongst its objectives the testing of a relatively detailed model of the repository vault. The geosphere submodel specification for Level 1a does not differ from that of Level E, whereas the near-field specification is considerably more complex for Level 1a than for Level E [2]. For this reason, most of the modelling differences amongst the participants relate to the vault. This Section contains general observations relating calculated release rates from the vault to the modelling approach employed.

A first observation relates to the similarity in results between participants A, B, E, and J. Participants A (EMOS code) and B (JAERI code) modelled the vault as a reaction tank, that is, radionuclide transport was not explicitly modelled in the vault itself. On the other hand, participants E and J used two different versions of the LISA code, which includes a finite-difference submodel for the vault. As noted in Section 3.2, the global agreement of results from these three codes, which have been developed independently, contributes to their verification.

Participant F had to adapt the specification in order to have an analytical expression in Laplace space. This participant has replaced the specified trapezoidal pulse arising from the convolution of matrix and drum degradation by a Gaussian function. As noted in Section 3.6, solubility limits were applied by considering the period corresponding to one-half of the solubility value. The modifications introduced do not, however, appear to have affected the results, apart from a "corner-of-the-pulse" effect, which is clearly explained in Annex B of the report. This effect is most evident for the vault release rate in DETRUN2 at 100 years. Globally, results for participant F agree with those for participants A, B, E, and J.

Participant H has modelled transport explicitly, and has included a diffusion term in the vault. Vault release rates for I-129 are high in DETRUN2, and this is consistent with the effect of diffusion, as explained in Section 3.5 of the report.

Participant I modelled the vault with a different approach: retention in the vault was not considered, and solubility limits were applied only in the vicinity of the container (i.e., not in the entire vault volume). Furthermore, in order to match the volume and flow through the vault with the specification, participant I had to introduce a flow bypass (see also Section 3.8). In addition, multiple-isotope solubility was not accounted for. I-129 release rates from the vault are relatively low for this participant, possibly owing to dispersion in the backfill.

Release rates from the vault calculated by participant K are systematically lower than the average rate of the other participants. This should be expected because this code does not contain a repository submodel, and the vault was simulated by extending the transport path (see Section 2.2). This participant did not consider solubility limits, although a comparison between concentrations and solubility limits was done in one of the vault segments, in order to answer question C2 (period of exceeding solubility limits).

Participant L has simplified the treatment of solubility limits by neglecting the multiple occurrence of isotopes of the same element, i.e., solubility limits are applied to each isotope separately. At the same time, this participant has used a detailed model of the vault, which includes a spatially distributed source in the vault with a spatial convolution to collect nuclides at the level of the vault floor. This concept yields a nuclide flow rate to the floor of the vault that reaches an approximately constant value over a long period. In contrast, the mixing-tank approach leads to the entire inventory being available for dissolution and transport in the first few hundred years, thus giving higher release rates at early times.

An additional delay has been introduced by explicit modelling of radionuclide transport through the 0.5-metre-thick floor of the vault.

These modelling differences for participant L are reflected in the results. For instance, in DETRUN3, participant L does not predict precipitation of U-234 at the vault floor. Furthermore, due to ingrowth from the large amount of U-238, U-234 release rates increase after 100,000 years. This local maximum is propagated through the geosphere, yielding a maximum dose from U-234 at about 400,000 years after repository closure, in contrast with the mixing-tank approach, which predicts a higher peak dose immediately after the breakthrough of U-234, at 100,000 to 130,000 years after repository closure. Despite these modelling differences, peak dose rates and times of peak dose for this participant are generally consistent with those of participants A, B, E, and J.

As observed in previous Sections, times of peak provided by participant D differ markedly from those provided by the other participants. The reasons for this are not clear, however. Participant D divided the vault into a series of 13 horizontal layers, each layer containing 1/13 of the total number of canisters. Canister failure was considered to occur at a constant rate, so that at time TDRUM all of the canisters have failed. The location of the canister that fails at each time was randomly selected. Matrix degradation was modelled as specified. The release rate of radionuclides from the matrix $S_i(t)$ was computed as the product of 1/TMATRIX and $m_i(t)$, where the latter term represents the mass evolution of the i^{th} radionuclide inside the waste matrix (see Annex B for further explanation).

3.8 Modelling of Dilution

As seen already, considerable differences in the results can be attributed to the different approaches employed to model the vault. The specification stated that groundwater flow velocity within the vault was to be computed as the product of the total vault cross-sectional area (23,000 square metres) and the Darcy velocity in the vault. The latter quantity was to be itself computed as the product of the Darcy velocity in the first layer of the geosphere and the FDARCYVLT factor. This computation yields, for DETRUN1, 2, and 3, the quantities 460, 0.23, and 18 cubic metres per year, respectively, for groundwater flow velocity in the vault. According to the specification, this flux was not to be diluted before the end of the geosphere, where the global FDILUT factor was to be applied. Participants A, B, E, and F were able to represent dilution in this way.

Participant H used a different approach to model dilution (see Annex B). This participant used the Darcy veolcity in the first layer of the geosphere to model dilution in the geosphere immediately after the vault (i.e., not at the geosphere/biosphere interface). Dilutions of 230, 23, and 127 cubic metres per year were obtained for DETRUN1, 2, and 3, respectively. These values are clearly different from those specified above (by a factor equal to FDARCYVLT), and this difference affects the results. Indeed, the different approach to modelling dilution can explain many of the differences in results between this participant and the average values of the others. For instance, in DETRUN2, despite the higher release from vault, this participant calculates relatively low total doses. In DETRUN1, release rates from the vault are generally low for this participant, as expected, with the exception of Tc-99 and I-129 at 1000 years, when relatively high values have been calculated. Use of a lower

flow rate (230 cubic metres per year instead of 460) results initially in a later release pulse, whereas at 1000 years, the other participants have already exhausted the Tc-99 and I-129 contents of the vault.

Participant C also introduced a dilution term at the vault/geosphere interface (see Section 3.9), and this is largely responsible for any differences in results between participant C and participants A, B, and E.

Participant I considered the total flow as defined by the specification, but a bypass was introduced before the vault, so that a smaller amount of water was simulated to flow through the vault itself. The bypass was recombined immediately after the vault, which results in a dilution of the flow from the vault. This approach leads to relatively low release rates from the vault for the less soluble elements, as can be observed in the results from this participant. I-129 release rates are also relatively low for this participant, possibly due to dispersion in the backfill.

Participant L used the gallery area (i.e., the effective vault cross-sectional area) rather than the total vault cross-sectional area in the final iteration, which gives rise to a dilution factor of about 2, as discussed in Annex B. Participant J also used the effective vault cross-sectional area.

3.9 Differences in Interpretation of the Case Specification

The Level 1a case specification left room for different interpretations. As just one example, some participants considered it inconsistent to use the effective vault volume for computing radionuclide retention and precipitation, and to use the total vault cross-sectional area to compute water flow (as specified): this led them to simulate the system in a different manner than implied by the case specification. In order to appreciate the significance of these different approaches, it was decided to retain in the analysis one set of results from the first iteration (contribution C), that was revised in the second iteration (contribution J). The differences in results between participant C and the cluster A, B, and E are due to the use of three assumptions:

(1) the use of effective vault porosity to compute radionuclide retention in the vault,

(2) the use of total vault cross-sectional area to compute water flow in the vault, and

(3) the assumed ratio of water flow in the geosphere to water flow in the vault.

The results from participant C and from the first iteration of participant E were very similar, as the two participants had used different versions of the same code. Thus, the differences in results between participant C (first iteration) and those from the second iteration of participant E can be attributed to different interpretations of the specification. These differences can be significant, and in the principal

component analysis (Figs. 3.1a-b), the two sets of results differ by more than one standard deviation. In particular, release rates from the vault differ on average by about a factor of 2. Since this factor is approximately constant for the three deterministic runs, it can be attributed to the use by participant C of the effective vault area in place of the total vault area to model dilution. The relative differences in calculated doses are much greater. For example, peak dose rates and total doses for DETRUN2 are generally 100 times lower for participant C than for participant E, again reflecting the effect of dilution at the vault/geosphere interface.

3.10 Stochastic Results

The stochastic results are illustrated in Fig. 3.6 (pages 28-29). Analysis of these plots reveals a variation in the results of about two orders of magnitude - excluding results for participant K - which becomes three orders of magnitude if participant K is included. This variation is relatively large when compared to that in the PSACOIN Level 0 and Level E exercises (typically a factor of about 2).

Unlike the results for Level 0, it is not possible here to correlate the variation in the mean dose to the number of runs. For example, for participant D, who calculated the largest means and standard deviations and performed 100 runs, the effects of modelling differences most likely dominate the effects of sample size. The same can be said for participant K, whose relatively low predictions at the earliest time point are not due to sample size (25 runs), but to the different conceptualisation of the vault (see Section 3.7).

The relatively low predictions by participant H for mean dose probably result from the assumptions concerning dilution (see Section 3.8). This effect appears less severe for the first time point, possibly due to the compensating effect of modelling diffusion in the vault, which is explicitly considered by this participant (see Section 3.5).

Relatively low results for mean dose by participant C are consistent with the use of effective vault cross-sectional area (lower flows), as explained in Section 3.9.

For participant L, it appears that data variability in the geosphere masks the effect of differences attributable to the modelling approach employed. In the deterministic results, this participant exhibited considerable differences in the vault (lower delayed releases due to more detailed modelling of the vault). As discussed previously, participant L's results for total dose (deterministic runs) are influenced by his prediction of later times of peak dose. This difference appears to be completely compensated for by the effects of input data variability, and participant L's predictions for mean dose agree with those of participants A, B, E, and J.

Mean dose predictions by participant I are also relatively low, indicating that the modelling differences identified are not compensated for by the effects of input data variability.

The results for standard deviation are difficult to interpret. This is mainly because the standard deviation depends upon the mean; when the means

vary over several orders of magnitude, possible effects due to sample size are masked. Participant K may have reduced the total variance of the exercise by holding constant the radionuclide retention factors in the stochastic runs (at their mean value).

3.11 Modelling Bias and Data Uncertainty

The main objective of the Level 1a exercise is, for one specific case, to evaluate te magnitude of differences arising from the use of different modelling approaches, and to compare these differences to output variations due to input parameter uncertainties. The preceeding Sections discuss in detail different modelling approaches and their effect on the calculated results. It is the aim here to compare this effect to the variance in results due to the (specified) uncertainty in input parameter values.

Fifty-two input parameters were treated as random variables, and their specified distributions are given in the case specification. Correlation between parameters has not been taken into account. Participants were requested to perform a Monte Carlo simulation of the disposal system and to give mean total dose rates and respective standard deviations at six specified times. For each participant, the standard deviations are taken as a measure of the variance in results due to input parameter uncertainty. To enable a rudimentary comparison of model uncertainty and parameter uncertainty for this exercise, the standard deviations were divided by their respective means to produce a nondimensional relative quantity. The ranges of resulting values at the six time points are given in Table 3.4: for each time, both the last and next-to-last values at the lower and upper limits of the range are given.

The impact of different modelling approaches can be estimated from the results of the three deterministic runs. Whereas values of input parameters have been selected to cover a wide range, their uncertainty, by definition, has no influence on the results of an individual deterministic run. Total dose rates at four selected times were usually given by all participants except G in answer to question C4 of the questionnaire. These results provide ten sets of data, each set containing up to eleven values of total dose rate. Only ten sets are available since the first two times in DETRUN2 have been neglected, all values except one being zero. The standard deviations in these sets are considered as measures of variance in results due to different modelling approaches. Table 3.5 contains the means and standard deviations of these ten sets of results, together with the ratio of the standard deviation and the mean in each case.

The ratios of standard deviation to mean from Tables 3.4 and 3.5 are compared in Fig. 3.11. Assuming the approach adopted in deriving this Figure has some validity, it can be seen that the relative effects of data variability are at least twice as great as those attributable to the use of different modelling approaches, except possibly at the earliest time point. A possible explanation is that at the earliest time, the absolute dose rates are relatively low and the dose curve is dominated by a few simulations where the doses are rapidly rising with time. Consequently, larger fractional variations between deterministic results arise - which can be considered to be attributable to differences in the various vault models employed - and model uncertainties are of increased significance. At other times, however, the effects of the geosphere mask any effects of the vault, and uncertainties due to data variability are relatively more significant.

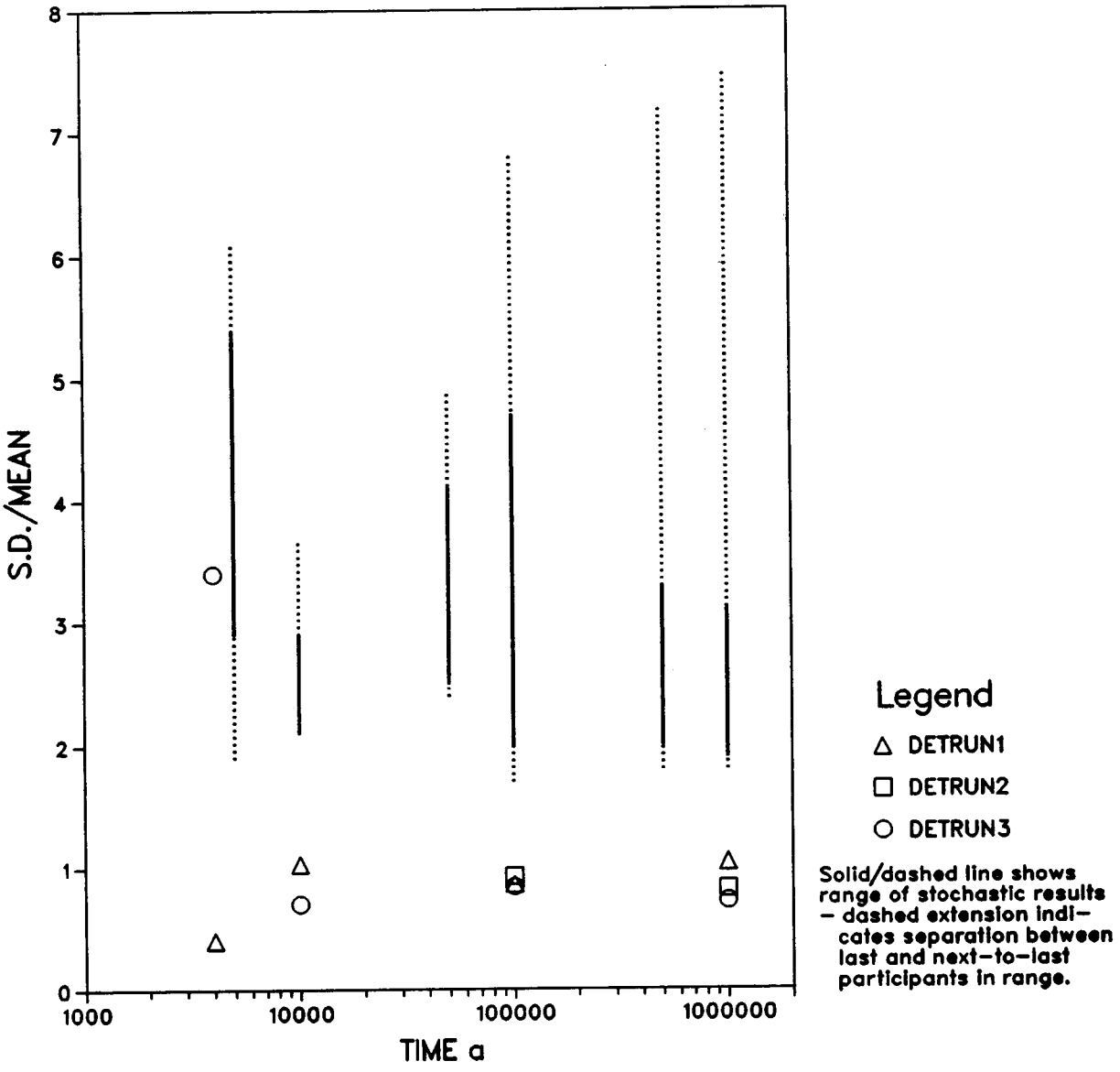
Table 3.4: Range of values obtained by dividing the standard deviation (SD) by the respective mean total dose rate at six times (a) for the eleven sets of results produced by Monte Carlo simulation. The corresponding participant letter is also shown. The SD and mean values can be found in Annex C.

	LOWER				UPPER			
	Last in range		Next-to-last		Last in range		Next-to-last	
Time	SD/Mean	Letter	SD/Mean	Letter	SD/Mean	Letter	SD/Mean	Letter
5.0E+03	1.9	D	2.9	J	6.1	F	5.4	E
1.0E+04	2.1	D,H	2.1	D,H	3.7	I	2.9	C,K
5.0E+04	2.4	J	2.5	H	4.9	D	4.1	E,F
1.0E+05	1.7	K	2.0	J	6.8	D	4.7	H
5.0E+05	1.8	J	2.0	C	7.2	D	3.3	I
1.0E+06	1.8	C	1.9	J	7.5	D	3.1	B

Table 3.5: Mean total dose rate (Sv/a), standard deviation (SD), and the quantity SD/mean from 11 contributions at four specified times (a) for each of the three deterministic runs.

	DETRUN1			DETRUN2			DETRUN3		
Time	Mean	SD	SD/Mean	Mean	SD	SD/Mean	Mean	SD	SD/Mean
4.0E+03	9.1E-05	3.6E-05	0.40	-	-	-	5.6E-07	1.9E-06	3.39
1.0E+04	3.3E-05	3.4E-05	1.03	-	-	-	2.3E-05	1.6E-05	0.70
1.0E+05	2.9E-06	2.5E-06	0.86	4.5E-06	4.2E-06	0.93	6.4E-07	5.4E-07	0.84
1.0E+06	9.3E-10	9.7E-10	1.04	6.1E-09	5.0E-09	0.82	2.9E-06	2.1E-06	0.72

Fig. 3.11: Comparison of standard deviations divided by means, showing the relative importance of model and data uncertainties in the PSACOIN Level 1a exercise. Data are from Tables 3.4 and 3.5 (see text for explanation).



The outcome of this comparison should be treated with caution. The Level 1a case is the first within the PSACOIN series where a degree of modelling freedom has been introduced by specifying processes to be modelled (previous exercises prescribed a set of equations to be solved). In order to simplify the interpretation of results, the specification still contained several modelling restrictions (that forced some of the participating codes to be used outside their stated domain of application). These constraints no doubt contributed to a larger conformity in the results than would have been expected without them, thereby artificially diminishing the observed impact of different modelling approaches. Furthermore, it is difficult to distinguish in this exercise between modelling uncertainties and coding errors. More importantly, when the results of several codes agree, it cannot necessarily be concluded that there is no model uncertainty. For example, it was stated in the specification that radionuclide transport through the two geosphere layers should be computed using one-dimensional models. Agreement between participants' results most certainly does not imply that one-dimensional modelling of the geosphere is without uncertainty; it merely implies that the use of one-dimensional models does not introduce significant differences under the conditions specified for this exercise.

There are, on the other hand, several discrepancies between the participants' results that can be attributed to different modelling approaches, and their impact is reflected in Fig. 3.11. In addition, some inconsistencies and ambiguities in the case specification were revealed during the course of the exercise. These are reflected by different interpretations of the specification, as discussed in Section 3.9. Their influence is included in the values of Table 3.5, as is the influence of (possibly) incorrect results. Removal of these influences would lead to even lower values in that Table.

Summing up, the PSACOIN Level 1a exercise is a first step toward quantification of the relative importance of model and data uncertainties. Restrictions and ambiguities in the case specification are suspected to have diminished artificially the influence of model uncertainty. Under the conditions of the exercise, however, it was found that the influence of data uncertainty was generally at least twice as great as that attributable to model uncertainty. Further thought is, however, needed on the methodology for comparison of uncertainties arising from the two sources.

4. CONCLUSIONS AND RECOMMENDATIONS

The PSACOIN Level 1a exercise represents a further step toward verification of the participating codes. In the specification for the Level 1a exercise, an attempt was made by two means to introduce more realism than was present in previous exercises:

- System complexity was increased, mainly by introducing a relatively complex structure for the repository vault. This is in accordance with a main conclusion from the Level E exercise, where the recommendation was made to pursue further code intercomparisons, with greater emphasis on the use of system models that are more representative of specific concepts for the disposal of radioactive waste.

- The case was described in terms of processes to be modelled rather than by a set of equations to be solved. Thus, some freedom in representing the case was introduced, although quite significant restrictions remained. The idea was to move participants a step further toward a real assessment, where artificial constraints would not exist, and where the available information has to be used together with the available modelling tools to represent the system as well as possible.

The principal objective of the Level 1a exercise was to evaluate the magnitude of the differences arising from the use of different modelling approaches, and to compare these with the variability in results due to input parameter uncertainties. Four main conclusions could be drawn from this exercise:

- With one exception, times of peak dose, as calculated by participants for the three deterministic cases, are in excellent agreement with each other - generally within 10% of the mean value.

- The bulk of results for peak dose rates show good agreement; the range of values generally varies over an order of magnitude. Given the level of freedom in modelling the case, this level of agreement is encouraging. In many cases, individual discrepancies can be attributed to different modelling approaches.

- Different assumptions were made mainly in modelling radionuclide releases out of the repository vault and dilution of contaminated flow during transit to the biosphere. In the context of this exercise, there are combinations of input parameter values for which diffusion significantly contributes to total release from the repository. Although differences in the representation of diffusion

from the repository contributed to differences in results, the concurrent use of different assumptions to model other processes - particularly dilution - makes the interpretation of such differences in results difficult. In contrast, differences in calculated radionuclide release rates from the repository could not be correlated with different approaches to representing solubility limitation.

- Under the conditions of the exercise, it was found that the variability in results attributable to data uncertainty was generally at least twice as great as that attributable to the different modelling approaches used by the participants. It is recognised, however, that the design of the case and the codes available to the participants probably limited the extent to which model uncertainty could be addressed. In addition, further thought is needed on the methodology for comparison of uncertainties arising from the two sources.

As noted above, the Level 1a exercise was a first step in estimating the relative importance of model uncertainties and data variability. The results from this limited study should, however, be interpreted with care. The case specification was such as to limit the range of modelling approaches that could be adopted, with a view to ensuring that the results obtained would be generally interpretable. Also, the constraints imposed in the case specification meant that some of the models were being used outside their stated domain of applicability, resulting in considerable effort being required by some participants to configure their models to meet the specification and to interpret the results obtained. Finally, the ranges of variability of the parameters were arbitrarily set and, for many parameters, the variability assigned was relatively large.

It is recommended, therefore, that future PSACOIN exercises should study in more detail the importance of modelling uncertainty relative to that arising from the variability of input data. In particular, it is considered that the case specifications should allow participants greater scope to adopt alternative modelling approaches.

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ANNEX A

PSACOIN Level 1a Intercomparison

Case Specification and Questionnaire

prepared by A. Nies (GSF/IfT)

C O N T E N T S

Note that the figure referred to as Figure 1 in this Annex is identical to that provided in the main text as Fig. 1.1, and this figure is therefore not reproduced in this Annex.

1 ACKNOWLEDGEMENT

The present work extensively benefits from a previous case specification prepared in several versions by Electrowatt Engineering Services (UK) Ltd.. Critical comments of great value have been received from Paul Kane and Steve Oldfield (Electrowatt Engineering Services (UK) Ltd.), and Timo Vieno (Technical Research Centre of Finland).

According to the organisational structure of PSACOIN, the case specification has been discussed, modified, and approved by the Level 1a Task Group. Aside from the author this Task Group comprises the following members:

Dan Galson (NEA Secretariat)
Jean-Marc Laurens (EWE/UK)
Ted Melnyk (AECL, Canada)
Andrea Saltelli (JRC/CEC)
Enrico Sartori (NEA Data Bank)

2 CASE SPECIFICATION

The site and disposal characteristics given in the following sections are of a hypothetical nature. Nevertheless, the attempt has been made to describe a realistic case that could be part of a true site-specific performance assessment.

2.1 GENERAL DESCRIPTION

The repository considered in the proposed case study is located deep underground on land within a geologic formation with relatively low permeability. The disposal formation (layer 1) is underlain by an aquifer (layer 2) which, some 20 km distant of the repository, crops out to a sub-surface Quaternary layer. Flow from layer 2 is diluted within a phreatic aquifer and enters the biosphere through a well. The situation under consideration is outlined in Figure 1.

Flow through the disposal formation is given as vertical in the downward direction and causes flow through the repository along its narrowest dimension. Along the aquifer, flow is essentially horizontal and remains within the formation's boundaries since the aquifer is underlain by an impermeable rock.

The vault consists of a central gallery with five disposal galleries branching to each side (see Figure 2). 500000 waste packages are stored in the disposal galleries as well as in the central gallery. The waste is encapsulated in a cement matrix and mild steel drums are used as containers. The remaining space in the vault is backfilled with cement.

The waste inventory comprises 13 nuclides, 5 of which are fission products and the other 8 belong to the Neptunium and Uranium-Radium decay chain. The chosen spectrum includes nuclides with various half-lifes,

solubilities, and sorption properties (see Tables 2 and 4). Some of the nuclides exist in the waste at the time of vault closure whilst others are created by decay only.

2.2 VAULT

Data about the vault geometry are indicated in Figure 2. The cross section of all galleries is 15m x 15m; the disposal galleries are 50m long while the central gallery has a length of 200m. The spacing between the disposal galleries is again 15m.

The cylindric drums are 1.1m high and 0.5m in diameter. They are stored in the galleries in a square-packing arrangement in each of 13 layers. 50cm between all natural rock walls and the containers, 20cm between the top of the highest container level and the ceiling of the vault, 50cm between the bottom of the lowest container level and the floor of the vault, and the remaining space between the containers and on the last about 12m of the central gallery are backfilled with cement. The situation is outlined in Figure 3.

Within the vault, the following processes are to be modelled:

- mobilization of radionuclides out of the waste packages
- precipitation of radionuclides when solubility limits are exceeded
- sorption of radionuclides by the cement in the vault as matrix and backfill material.

The mobilization of radionuclides out of the waste packages is prevented by two barriers: the cement matrix and the steel containers. Both barriers are described by lifetimes.

Container failure is modelled to occur at a constant rate between the beginning of the post-operational phase of the repository and the time TDRUM when the last container looses its integrity. The degradation of a cement matrix starts immediately after the corresponding container has failed. The matrix degradation is again modelled to occur at a constant rate given as the reciprocal of the time TMATRIX.

The fractional release rate can be computed by convolution of the container failure and the matrix degradation. The nuclide inventory is assumed to be homogeneously distributed within the waste packages so that the radionuclide mobilization can be obtained as the product of the fractional release rate and the nuclide inventory.

The vault is modelled as a homogeneous porous medium. Neglecting the containers' volume and possible empty voids, the porosity in the vault can be considered to be identical with the porosity PORVLT in the matrix and backfill cement. Soon after vault closure, the pore volume will be saturated with the water from the surrounding disposal formation. The time of the saturation process is not to be modelled, so that the pores in the vault are assumed to be water-filled from the beginning of the post-operational phase.

The sorption of the mobilized radionuclides is described by the distribution coefficients in Table 4. Only the matrix and backfill cement in the vault are considered to be sorbent. The remaining, unabsorbed part of the mobilized radionuclides is either in solution or, when solubility limits are exceeded, precipitates, forming a deposit.

Transport of radionuclides out of the repository is limited to the mobilized nuclides in solution. Flow through the vault is given as the product of the Darcy velocity within the vault and of a cross-section area of 200m • 115m (compare Figure 2). The Darcy velocity within the repository is obtained from that in the undisturbed formation, multiplied by the factor FDARCYVLT (see Table 3). The factor is modelled as a random variable, accounting for the unknown ratio of permeabilities in the disposal facility and formation.

2.3 GEOSPHERE AND BIOSPHERE

Radionuclides that have been released from the vault are transported vertically downward through the disposal formation toward the aquifer and, subsequently, along the aquifer to the Quaternary layer (see Figure 1). Velocities along both pathways are modelled as random variables, but constant along each of the two layers.

The flow rate within the two layers is kept to the same value as the flow rate through the repository, while dilution with additional flow is accounted for by the factor FDILUT described below. According to the continuity equation this restriction leads to artificially small cross-sectional areas of the transport pathway for certain input parameter values.

Nuclide transport through the two geosphere layers is to be computed using one-dimension models. Advection and dispersion are to be considered as transport mechanisms. During transport, the concentrations are reduced by sorption and diluted by dispersion effects. Sorption is modelled as a equilibrium linear process using KD-values (Table 4). The layers are assumed to be isotropic and dispersion is modelled by employing longitudinal dispersion lengths (see Table 3).

Contaminated flow from layer 1 is possibly diluted at the interface of layers 1 and 2, along layer 2, and within a phreatic aquifer at the end of layer 2. All these dilutions are modelled by one factor FDILUT (see Table 3) by which the concentrations at the end of layer 2 are to be divided. Only water with the resulting concentration is pumped from a well.

Biosphere modelling is reduced to a simple drinking water pathway. It is assumed that a well has been installed in the area where the aquifer crops out beneath the Quaternary layer. The dose rate to the critical group is computed as the product of diluted concentration, water consumption rate (see Table 1) and the dose conversion factors (see Table 2).

3 INPUT DATA

According to the objective pursued throughout the case specification, a set of hypothetical, yet realistic input data is proposed in this section. The data base is contained in Tables 1 to 4 and grouped in constant (Tables 1 and 2) and variable parameters (Tables 3 and 4).

Table 1 essentially contains information on the geometry of the vault and the waste containers together with the materials used. Also included is the water consumption rate indicating the annual consumption of contaminated well water per capita. The given values of total porosities are to be used for the computation of

- bulk densities out of the given densities of solids
- retardation factors out of the KD-values given in Table 4.

Further constant parameters are given as nuclide-specific data in Table 2. These include half-lives, total inventory, and dose conversion factors. According to the biosphere model, the dose conversion factors refer only to the radiological impact on adults of ingestion of contaminated well water.

Table 3 contains a description of the nuclide-independent random variables. Besides the container and matrix lifetimes, most of the given parameters characterize the conditions along the transport pathway. The parameter distributions have been chosen in a way to describe two geosphere layers of differing hydrogeological properties. The dilution factor FDILUT can be interpreted to account for the dilution of the contaminated flow along the pathway and by transversal dispersion, which is neglected in one-dimensional calculations.

In accordance with [1](p.233) the coefficient of hydrodynamic dispersion is obtained as the sum of the coefficients of mechanical dispersion and of molecular diffusion in a porous medium. The latter is called the effective diffusion coefficient in Table 3 and is not treated as a nuclide-specific quantity, but only as a nuclide-independent random variable. The coefficient of mechanical dispersion is computed as the product of the longitudinal dispersion length LDISPx and the fluid velocity v, which in turn is the quotient of the Darcy velocity VDARCYLx and the effective porosity PORLx.

Four generic types of parameter distribution have been employed, namely the uniform, loguniform, normal, and lognormal distributions. For each distribution type the given values A and B in Table 3 specify the range from which the sample is to be drawn. By definition, a random variable X has a loguniform (lognormal) distribution in the range from A to B if $\log_{10}X$ has a uniform (normal) distribution in the range from $\log_{10}A$ to $\log_{10}B$.

Consequently, for the normal and the lognormal distribution the given values A and B are to be interpreted as truncation values, i.e., no values must be sampled outside the range from A to B. The range limits are the 0.001- and 0.999-quantile, respectively. From these quantities

the mean m and the standard deviation s of a normal distribution are deduced as [2]

$$m = \frac{A+B}{2} \qquad \text{and} \qquad s = \frac{B-A}{6.18}$$

The mean and the standard deviation of $Y = \log_{10}X$, where X has a lognormal distribution, are computed with the same formula, but replacing A and B by $\log_{10}A$ and $\log_{10}B$, respectively.

Element-specific KD-values and solubility limits are treated as independent random variables. The distribution of the KD-values is loguniform whilst that of the solubility limits is lognormal. The range limits A and B for the solubility limits are obtained by multiplying the values in Table 4 with 1/100 and 100, respectively. Similarly, the range limits A and B for the KD-values are computed by multiplying the values in Table 4 with 1/10 and 10.

15 nuclide-independent and 37 element-specific parameters make a total sum of 52 random variables in the proposed case study.

4 EXAMPLE RESULTS

Example results are not included in this report in order to make the intercomparison a blind exercise. It is expected that analysis results computed by the participants will spread considerably, due to different modelling approaches. In order to separate the effect of these model uncertainties from the impact of input parameter uncertainties, deterministic system simulations are part of the exercise.

More specifically, three deterministic system simulations are requested. Input parameter values for the random variables have been chosen in a way to cover a wide range of possible outcomes (see Table 5). The values of all constant parameters are given in Tables 1 and 2.

For the KD-values (resp. solubility limits), the values of Table 4 are to be taken for DETRUN3, 1/10 (resp. the 100-fold) of these values for DETRUN1, and the 10-fold (resp. 1/100) of these values for DETRUN2. To give an example, the KD-value of Uranium in the vault is 10 l/kg for DETRUN3, 1 l/kg for DETRUN1, and 100 l/kg for DETRUN2, while the solubility limit of Uranium is 10^{-5} mol/l in DETRUN3, 10^{-3} mol/l in DETRUN1, and 10^{-7} mol/l in DETRUN2.

5 REFERENCES

[1] J.BEAR: Hydraulics of Groundwater. McGraw-Hill, New York 1979

[2] R.L.IMAN, M.J.SHORTENCARIER: A FORTRAN 77 Program and User's Guide for the Generation of Latin Hypercube and Random Samples for Use With Computer Models. Sandia Report SAND83-2365, Albuquerque, March 1984

TABLE 1: DESCRIPTION OF PARAMETERS TO BE TREATED AS CONSTANTS

Cross section of all galleries	:	15m x 15m
Length of disposal galleries	:	50m
Length of central gallery	:	200m
Number of disposal galleries	:	10
Spacing between disposal galleries	:	15m
Total number of waste packages	:	500000
Height of containers	:	1.1m
Diameter of containers	:	0.5m
Material of containers	:	Mild steel
Matrix material	:	Cement
Backfill material	:	Cement
Cement density *)	:	2500 kg/m^3
Rock density *) in layer 1	:	2600 kg/m^3
Rock density *) in layer 2	:	2500 kg/m^3
Total porosity within the vault	:	0.20
Total porosity in layer 1	:	0.35
Total porosity in layer 2	:	0.40
Water consumption rate	:	0.8 m^3/year

*) The given values are to be interpreted as densities of solids.

TABLE 2: NUCLIDE-SPECIFIC DATA

NUCLIDE	HALF-LIFE (y)	TOTAL INVENTORY (kg)	DOSE CONVERSION FACTOR (Sv/Bq)
C - 14	5.7 E 03	1	5.7 E-10
Ni- 59	8.0 E 04	100	5.7 E-11
Se- 79	6.5 E 04	1	2.4 E-09
Tc- 99	2.1 E 05	50	3.9 E-10
I -129	1.6 E 07	100	6.7 E-08
Np-237	2.1 E 06	50	1.1 E-06
U -233	1.6 E 05	0	7.8 E-08
Th-229	7.3 E 03	0	9.5 E-07
U -238	4.5 E 09	100000	6.9 E-08
U -234	2.4 E 05	10	7.7 E-08
Th-230	7.7 E 04	0	1.4 E-07
Ra-226	1.6 E 03	0	3.6 E-07
Pb-210	2.2 E 01	0	1.5 E-06

TABLE 3: DESCRIPTION OF PARAMETERS TO BE TREATED AS RANDOM VARIABLES

NAME	UNITS	DISTRIBUTION	VALUE A	VALUE B	PARAMETER DEFINITION
TDRUM	y	normal	100	500	maximum container lifetime
TMATRIX	y	uniform	200	400	matrix degradation time
PORVLT	-	uniform	0.10	0.20	effective porosity in vault
PORL1	-	uniform	0.05	0.10	effective porosity in layer 1
PORL2	-	uniform	0.20	0.25	effective porosity in layer 2
VDARCYL1	m/y	uniform	0.001	0.01	Darcy velocity in layer 1
VDARCYL2	m/y	uniform	0.1	1	Darcy velocity in layer 2
FDARCYVLT	-	loguniform	0.01	2	Ratio of Darcy velocity in vault to that in layer 1
LPATH1	m	normal	90	110	pathlength through layer 1
LPATH2	m	normal	17000	23000	pathlength through layer 2
CDIFF1	m^2/y	normal	0.002	0.005	effective diffusion coefficient for layer 1
CDIFF2	m^2/y	normal	0.005	0.02	effective diffusion coefficient for layer 2
LDISP1	m	uniform	1	10	longitudinal dispersion length in layer 1
LDISP2	m	uniform	50	500	longitudinal dispersion length in layer 2
FDILUT	-	loguniform	10^{-5}	10^{-3}	dilution factor

TABLE 4: ELEMENT-SPECIFIC DATA

ELEMENT	KD-VALUES IN l/kg			SOLUBILITY LIMITS
	VAULT	LAYER 1	LAYER 2	IN mol/l
C	0.5	1	0.5	1.0 E-05
Ni	5	1	5	1.0 E-05
Se	1	1	1	1.0 E-02
Tc	0.1	0.5	0.5	1.0 E-05
I	0	0	0	1.0 E-00
Np	50	10	10	1.0 E-07
U	10	5	1	1.0 E-05
Th	1000	500	1000	1.0 E-08
Ra	1	1	5	1.0 E-04
Pb	5	10	100	1.0 E-05

TABLE 5: PARAMETER VALUES USED IN THE DETERMINSTIC SIMULATIONS

NAME	UNITS	DETRUN1	DETRUN2	DETRUN3
TDRUM	y	100	500	300
TMATRIX	y	200	400	300
PORVLT	-	0.10	0.20	0.15
PORL1	-	0.05	0.10	0.075
PORL2	-	0.20	0.25	0.225
VDARCYL1	m/y	0.01	0.001	0.0055
VDARCYL2	m/y	1.0	0.1	0.55
FDARCYVLT	-	2	0.01	0.1414
LPATH1	m	90	110	100
LPATH2	m	17000	23000	20000
CDIFF1	m^2/y	0.005	0.002	0.0035
CDIFF2	m^2/y	0.02	0.005	0.0125
LDISP1	m	1	10	5.5
LDISP2	m	50	500	275
FDILUT	-	0.001	0.00001	0.0001

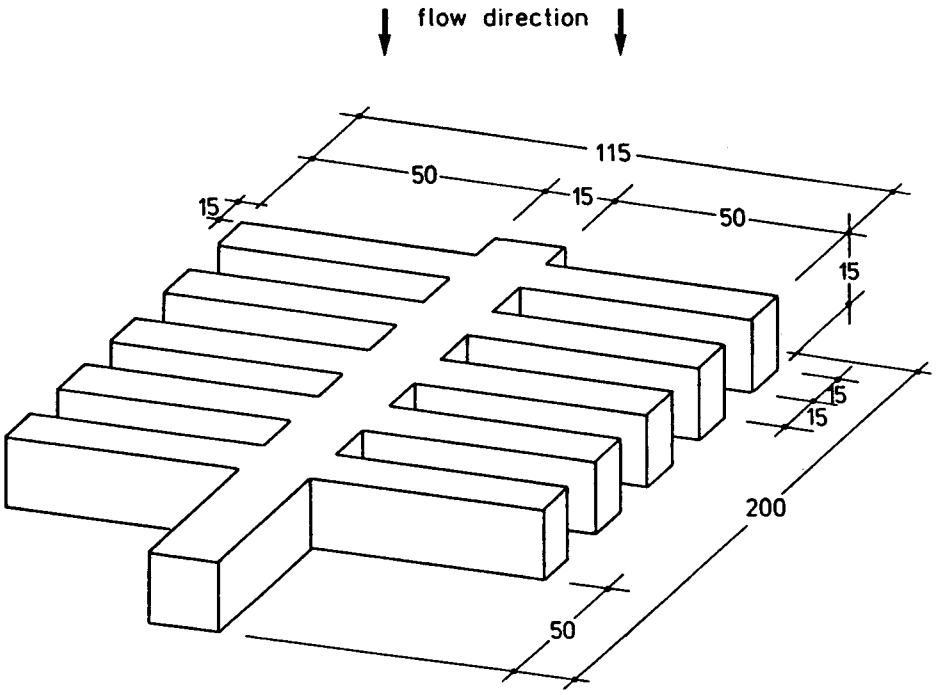

Figure 2 : Configuration of vault

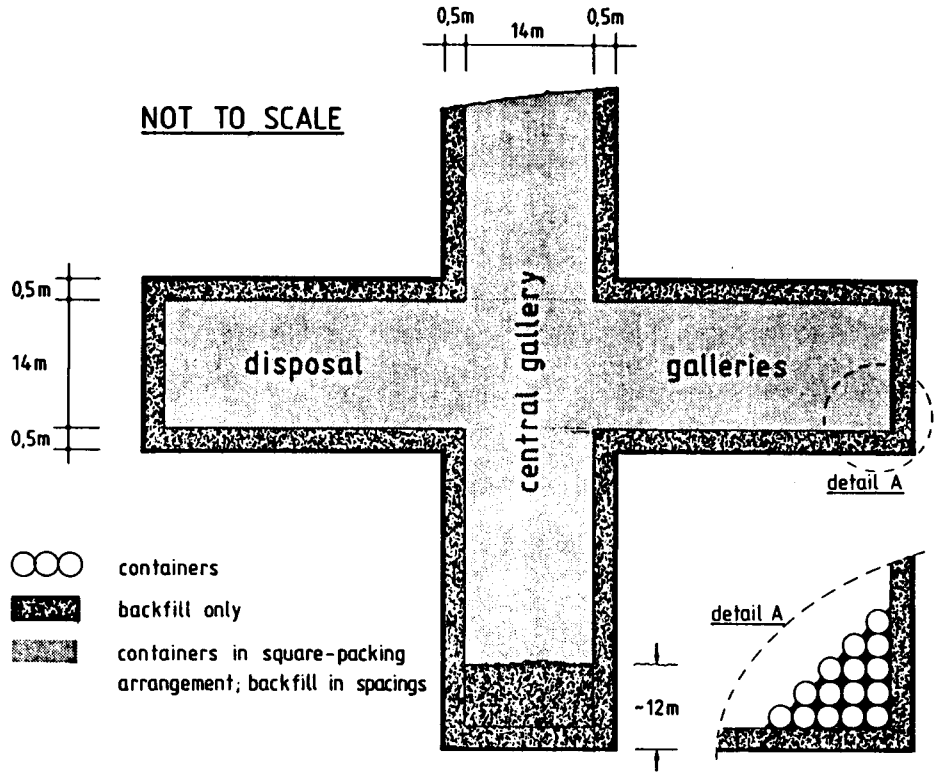

Figure 3: Storage and backfill areas in the vault

ANNEX: QUESTIONNAIRE FOR PSACOIN LEVEL 1A

GENERAL NOTES

In the light of the experience with previous PSACOIN exercises the questionnaire has been shortened. The remaining questions are to be answered by each participant in order to make the statistical analyses of the NEA Data Bank possible. It is, of course, appreciated if you provide additional information like figures, problems encountered, etc.

Because the Level 1a case specification describes processes rather than equations a considerable variance in the analysis results is expected. The effect of these model uncertainties will be studied by comparison of the results of deterministic simulations. In order to get a first idea where different models or assumptions have been introduced, section B is included in this questionnaire.

Owing to the expected variance in results, Section C with deterministic results is extended and Section D with stochastic results is just one Table. Possibly this questionnaire will be modified after the first iteration of running the case.

A cut-off time of one million years has been agreed upon for all Level 1a calculations. This means that, in question C2, you have to enter " > 1000000 " in column "End" whenever one of the radionuclides still exceeds its solubility limit at one million years. Similarly, in question C3, the time of peak dose is only to be quantified within the time span up to one million years.

As with the previous questionnaires please note the following points:

1. Please use separate copies of this questionnaire if you wish to submit more than one set of results.

2. The numbers given in the headlines of Tables C1, C4, and D1 are to be interpreted as times in years.

3. Specified times refer to the time of vault closure.

4. In the questions, 'dose' means "annual effective dose equivalent", and 'total dose' means "dose summed over all nuclides".

5. Radionuclide dose values of less than 10^{-15} Sv/a may be considered zero.

6. Please enter all your numbers with one digit after the point (Example: 1.2E-03).

SECTION A: GENERAL INFORMATION ABOUT PSA CODE

A1. Name and address of contact person

A2. Name of code

A3. Version Number and Date

A4. Sampling technique

A5. Number of runs

A6. Number of time steps per run (if applicable)

SECTION B: DESCRIPTION OF MODELS AND ASSUMPTIONS

Participants are encouraged to give a 1-2 page summary of their model approaches. The information provided should contain describing equations and other detailed information rather than statements like "analytical solution". Of particular interest are simplifications, modifications, or approximations which were necessary when applying your code. Did you make additional assumptions not mentioned in the specification, or did you fail to follow any prescriptions of the specification? These and related questions should be answered in the summary. Please supply your summary at the end of this questionnaire.

SECTION C: DETERMINISTIC RESULTS

C1. Radionuclide release rates (mols/a) out of vault at selected time points (a)

NUCLIDE	DETRUN1		DETRUN2			DETRUN3		
	100	1000	100	1000	1000000	100	1000	10000
Tc- 99								
I-129								
Np-237								
U-238								
U-234								

C2. Period of exceeding solubility limits

Nuclide	Period of exceeding solubility limits					
	DETRUN1		DETRUN2		DETRUN3	
	Begin	End	Begin	End	Begin	End
Tc- 99						
Np-237						
U-238						

C3. Peak dose (Sv/a) and Time of peak (a)

Nuclide	DETRUN1		DETRUN2		DETRUN3	
	Peak dose	Time of peak	Peak dose	Time of peak	Peak dose	Time of Peak
Tc- 99						
I-129						
Np-237						
U-238						
U-234						

C4. Total doses (Sv/a) for selected time points (a)

Run	4000	10000	100000	1000000
DETRUN1				
DETRUN2				
DETRUN3				

SECTION D: STOCHASTIC RESULTS

D1. Statistics of total dose (Sv/a) at selected time points (a)

Statistic	5000	10000	50000	100000	500000	1000000
Mean dose						
Standard deviation						
Lower 95% confidence limit on estimate of mean dose						
Upper 95% confidence limit on estimate of mean dose						

Please indicate the equation with which you have calculated the confidence limits or, if necessary, give a reference.

ANNEX B

Descriptions of Participating Codes

Section B of the PSACOIN Level 1a questionnaire encouraged all participants to provide a 1-2 page summary of their modelling approaches, and any assumptions made in implementing the case specification with their code (see Annex A of the report). Participants were also asked to describe any simplifications, modifications, and approximations that were made in applying their code to the exercise. All of the participants provided such information on their codes, and the information provided is included in this Annex, in largely unedited form. Most of the participants provided the suggested two pages, but a few participants provided extremely detailed responses to Section B of the questionnaire. This detailed information proved extremely useful to the Case Results Analysis Task Group (the editors of this report), and it is therefore included in its entirety here.

Code summaries are provided for each of the 12 contributions discussed in this report. The summaries are ordered according to the identifying letter attributed to each contribution in Section 1 of the report (see Table 1.1). The name and address of a contact personn for each code is provided immediately after the contents list.

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VAULT

Mobilization of radionuclides out of the waste packages is modelled in exactly the manner prescribed in the case specification. It is assumed that the mobilized nuclides are homogeneously distributed within the vault. In principle there are three forms in which mobilized nuclides are present in the vault: they are either in solution, or they are sorbed, or, when solubility limits have been exceeded, they precipitate, forming a deposit.

The volume of solution present in the vault (V_L = 31.500 m^3) is calculated as the product of the total volume of the vault (157.500 m^3) and the total porosity within the vault (0.20). Note that the random variable PORVLT is not used in our modelling. The mass of sorbent present in the vault (m_S = 315.000.000 kg) is obtained as the product of cement volume in the vault (157.000 m^3 - 31.500 m^3) and the cement density (2500 kg/m^3). With these two quantities and the element-specific k_D-value and solubility limit L we obtain the maximal number of particles that can be in solution resp. sorbed within the vault:

$$I_{L,max} = V_L \cdot L \qquad \text{(maximal solved moles)}$$

$$I_{S,max} = m_S \cdot L \cdot k_D \qquad \text{(maximal sorbed moles)}$$

Whenever the total amount of moles I_g of an element present in the vault is greater than the sum of $I_{L,max}$ and $I_{S,max}$, precipitation takes place, and the solved part a of I_g is given as $I_{L,max}/I_g$. Otherwise no precipitation takes place and the solved part a is calculated as

$$a = 1 / (1 + m_S \cdot k_D / V_L)$$

With these quantities the nuclide-specific release rate R_i out of the vault is calculated as

$$R_i = a \cdot I_{g,i} \cdot S_L / V_L \quad \text{(moles/year)}$$

where S_L is the flow rate through the vault, calulated according to the specification, and $I_{g,i}$ is the total amount of mobilized moles of nuclide i.

GEOSPHERE AND BIOSPHERE

Transport of released radionuclides is calculated with a modified version of the Swiss finite difference code TROUGH. The modifications include a complete reconstruction of all input parts of the code to be run within the EMOS executive. In addition, a game-specific optimization of the discretization in space and time has been introduced.

To be specific, the length dx of the finite difference cells is chosen to be as large as possible up to a limit of the double of the actual dispersion length in each layer. Subsequently, the time step is chosen to be as large as possible up to a limit of

$$2 \cdot dx \cdot R_{f,min} / v$$

where v is the water velocity and $R_{f,min}$ is the minimum of all actual retardation factors.

The results calculated by our TROUGH-implementation are nuclide-specific activity concentration and the end of layer 2. These are subsequently transformed to dose rates according to the specification.

Participant: B Code: JAERI Organisation: JAERI/Japan

The model for simulating the release rate of radionuclides from a vault is newly incorporated into the PSA code called JAERI(tentative) to treat the Level 1a Exercise. The other models used in the JAERI code remain unchanged.

VAULT MODEL

The new vault model is based on the following assumptions:
All radionuclides are immediately dissolved and the concentration of each nuclide becomes uniform when the nuclide is released from waste packages. Linear sorption equilibrium is established instantaneously. A specified solubility limit is applied to each element in the vault in such a way that the simultaneous presence of different isotopes of the same element is separately taken into account in each chain.

The formulation of the VAULT model is summarized below:

Fractional release rate

The fractional release rate f(t) of a radionuclide from waste packages is given by the following equations depending on the time with respect to the maximum container lifetime (TDRUM) and the matrix degradation time (TMATRIX), where TDRUM is assumed to be smaller than TMATRIX.

1) $t < TDRUM$

$$f(t) = \frac{t}{TDRUM * TMATRIX}$$

2) $TDRUM < t < TMATRIX$

$$f(t) = \frac{1}{TMATRIX}$$

3) $TMATRIX < t < TDRUM + TMATRIX$

$$f(t) = \frac{1}{TDRUM} + \frac{1}{TMATRIX} - \frac{t}{TDRUM * TMATRIX}$$

4) $TDRUM + TMATRIX < t$

$$f(t) = 0$$

where t is the time after vault closure.

In the case when TDRUM is greater than TMATRIX, the release rate is also given by the above equations, but TDRUM and TMATRIX are replaced by each other.

Release rate from the vault

The release rate from the vault Oi(t) is given by the following equations:

$$Oi(t) = Ri * Ii(t)$$

$$Ri = \frac{1}{1 + Ms*kdi/Wp} * \frac{vl * S}{Wp}$$

$$\frac{dIi(t)}{dt} = - \lambda i\ Ii(t) - Ri\ Ii(t) + f(t)\ Mi(t) + \lambda i\text{-}1\ Ii\text{-}1(t)$$

$$\frac{dMi(t)}{dt} = - \lambda i\ Mi(t) + \lambda i\text{-}1\ Mi\text{-}1(t)$$

where

Ri	:	release rate of i-th radionuclide in the chain,
Ms	:	mass of cement,
kdi	:	distribution constant of i-th radionuclide in the chain,
Wp	:	amount of porewater,
vl	:	Darcy velocity of the ground water through the vault,
S	:	cross-section area,
Ii(t)	:	total amount of i-th solved and sorbed radionuclide in the chain,
Mi(t)	:	inventory of i-th radionuclide in the chain,
λi	:	decay constant of i-th radionuclide in the chain.

GEOSPHERE MODEL

The geosphere model is the same as the model used in PSACOIN Level E except that the model used here includes a diffusion term. The flux of the 4th and 5th chain members, Ra-226 and Pb-210, are calculated assuming secular equilibrium.

BIOSPHERE MODEL

The biosphere model is as follows.

$$Di(t) = Fi(t)*w*Dfi*FDILUTE* \frac{1}{VDARCYL1*VDARCYVLT*S}$$

where

Di(t)	:	annual dose of i-th radionuclide in the chain,
Fi(t)	:	flux from geosphere of i-th radionuclide in the chain,
w	:	water consumption rate,
Dfi	:	dose conversion factor of i-th radiocuclide in the chain,
FDILUTE	:	dilution factor,
VDARCYL1	:	Darcy velocity in the first layer,
VDARCYVLT	:	ratio of Darcy velocity in vault to that in the first layer,
S	:	cross-section area.

Participant: C Code: LISA-1A/CI Organisation: CIEMAT/Spain

This paper describes briefly the equations of each submodel of the LISA1a code and the processes that are represented in it.

VAULT

According to the LEVEL-1a specifications for this submodel, the waste in a cement matrix is included in a steel container. The mobilization of radionuclides out of the packages depends on the rate of container failure considered to be constant and the matrix degradation that occur also at a constant rate. The fractional release rate is modelled through the convolution of both processes, taking into account that TDRUM is the time for the last container failure and TMATRX is the time in which the complete dissolution of the matrix is supposed to occur. Both times are represented by distributions in the input file and either of them can have values smaller or greater than the other.

After the element releases out of the container, the following processes are modelled in the vault submodel:

- Advective transport.

- Radionuclide precipitation, after reaching the respective solubility limits.

- Chemical retention, controled by a linear isotherm.

- Radioactive decay (both in dissolved and precipitated phases).

The transport equation within the vault submodel is solved by the finite difference method with a explicit of the first order. The equation includes advective transport , chemical retention, radioactive decay (even inside the cement matrix) and a source term.

The precipitation-solution processes are evaluated for different times within each run and for all the isotopes of a nuclide, that is, the multiple isotope precipitation. Because of this, the two actinide chains have been changed into a single one with the help of a dummy nuclide . The code tests for several times the mass balance equation of the radionuclides either in solution , or as sorbed, precipitate and matrix phases. Then this amount is fitted with the amount of elements that have left the vault by that time and the whole inventory (both with radioactive decay).

FAR FIELD

LISA1a code has incorporated TROUGH code to represent the far field submodel. TROUGH is a 1-dimensional code in finite

differences scheme that solves the transport equation of radionuclides in groundwater with the Crank-Nickolson method, in a multilayered medium. It was incorporated in LISA_K4 code for the LEVEL-E by A. Saltelli maintaining the same configuration in LISA1a code.

According to the LEVEL-1a specifications the submodel for the far field subsystem represents the following processes:

- Advection and dispersion.
- Sorption with a equilibrium linear process.
- Dilution by dispersion effects.
- Radioactive decay.

BIOSPHERE

LISA1a code follows the LEVEL-1a specifications in this submodel, evaluating the dose rate to the critical group as the product of diluted concentration, water consumption rate and the dose conversion factors.

PROBLEMS ENCOUNTERED

LISA1a code has been implemented in the computer system of the CIEMAT. There are three VAX computers in a cluster configuration, two of them being VAX-8350, biprocesors with 32Mb central memory, and the other one is a VAX-11/785, with a floating point accelerator and 14 Mb central memory.

There were several problems with the implementation of the computer code because this version was developed at first on a AMDAHL computer. For this reason several minor computer modifications were introduced in the code in order to fit it to the actual CIEMAT computer system.

LISA1a code computes the space grid points as a function of the dispersion length. Due to the actual values of this parameter in relation to the path lenght values in the input file for LEVEL-1a, a great number of grid points is generated. There are also a high number of time points discretised because these points are dependent of the space step in order not to translate the information more than one grid point between two time points. All this implies a high CPU time consumption, exactly 4 days and 12 hours for our test case with 100 probabilistic runs and 3 deterministic runs.

The only modification that has been introduced in the input file for LEVEL-1a is to consider the Pb-210 half-life as 1.000E+07 years instead of 2.200E+01 years.

Question C.4. in the Questionnaire does not include the total dose(Sv/y) for the first deterministic run for 1.0E+05 and 1.0E+06 years. The reason of this is that these times exceede the cut-off time and doses are not calculated beyond this limit.

Participant: D Code: SIMPAR-2.0 Organisation: ETSII/Spain

SIMPAR comprises the following programs:

a) LHSCTN for the generation of samples,
b) VAULT-CTN for the simulation of the near field,
c) TROUGH-1D as far field model,
d) BIO-1A for the biosphere calculations, and
e) POST-1A for the post-processing of stochastic simulations.

1.- SAMPLE GENERATION

LHS (Ref.1) is a program commonly used to generate samples from the distribution functions characterizing parameter uncertainties. LHSCTN is a version of LHS in which new distributions have been added and some error-checking routines have been optimized.

2.- SIMULATION OF THE NEAR FIELD

The model described hereby (Ref.2) is the result of modelling the near field proposed in the PSAC Level-1a exercise specifications, and is structured taking into account:

a) discretization of the vault,
b) container failure,
c) source term
   . matrix degradation
   . radioactive decay
d) one dimensional transport equation,
e) precipitation phaenomenon.

a) The vault is discretized into a number of cells equal to the number of canisters stored in the repository. Taking into account the canister allocation inside the repository, the water flow direction, and knowing that the diffusion phaenomenon is not considered, it is possible to cluster thirteen down contiguous cells belonging to different layers into a transport column (see figs 1,2).

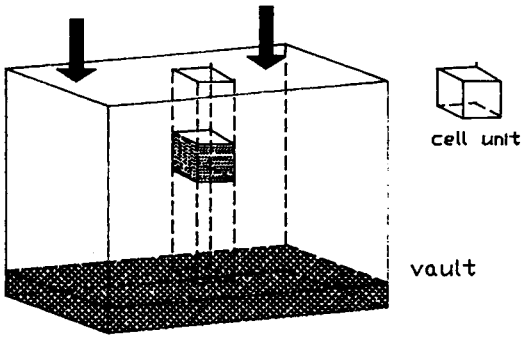


Figure 1.- Near Field Discretization.

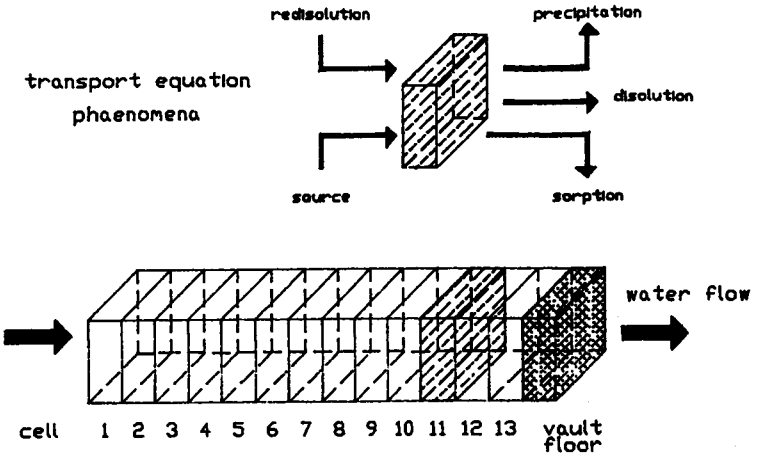


Figure 2.- Transport Column.

b) Canister failure is modelled to occur at a constant rate so that at time T_{DRUM} all the canisters have failed.

A subroutine, MATORD, randomly selects the allocation of the canisters that have been failing. A failure time is associated to each canister in the following way:

$$Tr(k) = NRAN * Tx \qquad \text{(eq. 1)}$$

where,

NRAM ..... integer random number between 1 and 500000
Tx ..... T_{DRUM} / 500000

These data are stored in a binary file from which the data will be read later.

Thus, for example, a column of the vault could have the following distribution of failure times, supposing a value for T_{DRUM} equal to 300 y :

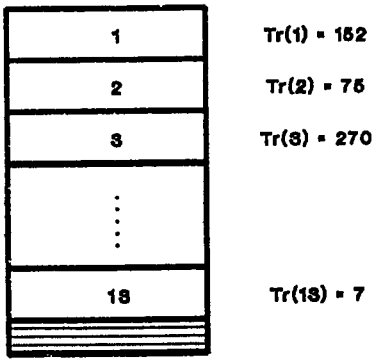


Figure 3.- Failure times for a transport column.

c) The source term for each cell is obtained considering the two following processes:

1. BATEMAN EQUATION for the five members of the same decay chain

2. MATRIX DEGRADATION between Tr(k) (cell failure time) and Tr(k) + T_{MATRIX}, at a constant rate $1/T_{MATRIX}$.

In these conditions, the isotopic inventory evolution inside a cell is:

$$\delta m_i(t)/\delta t = -\lambda_i m_i(t) - S_i(t) + \lambda_{i-1} m_{i-1}(t) \qquad \text{(eq.2)}$$

where, $S_i(t)$ ..... $1/T_{MATRIX} * m_i(t)$

and the expression for $m_i(t)$ will be:

$$m_i(t) = BATMAN(m_i(0)) * \exp(-1/T_{MATRIX} * t) \qquad \text{(eq.3)}$$

Therefore, the source term would have the following expression:

$$\begin{array}{lll} S_i(t) = 0 & t < Tr(k) & \\ S_i(t) = 1/T_{MATRIX} * m_i(t) & Tr(k) \leq t \leq Tr(k) + T_{MATRIX} & \text{(eq.4)} \\ S_i(t) = 0 & t > Tr(k) + T_{MATRIX} & \end{array}$$

d) Radionuclides are transported in solution with the water flow, which is obtained as follows:

$$\Phi(m^3/y) = V_D * STOT \qquad \text{(eq.5)}$$

where, STOT ..... 200 x 115 m^2
V_D ..... vault ground water velocity

The vault TRANSPORT equation (Ref.3) is considered one-dimensional, including advective term, radioactive decay and source term, using a explicit scheme to solve it.

The stability condition for the transport equation is the following (Ref.4)

$$\alpha \Delta t/\Delta x \leq 1 \qquad \text{(eq.7)}$$

where .. α .. is the coeficient of the next equation :

$$\partial C/\partial t + \alpha\ \partial C/\partial x = 0 \qquad \text{(eq.8)}$$

e) For each cell and each time, the solubility limit (SL) of each element is compared to the element concentration (C), if SL_e is lower than $C_e(t,x)$, the difference between these two quantities precipitates in that cell. This quantity is considered in the balance for the next time step, where decay is also taken into account.

The time at which each element starts to precipitate as well as the time when the element concentrations begin to be lower than SL_e are written on the output file.

3.- SIMULATION OF THE GEOSPHERE

The TROUGH-1D code (Ref.5) has been used to simulate the transport along the two layers of the geosphere .

Within the SIMPAR procedure, the input files for TROUGH-1D are built taking into account the vault output file and the geosphere specifications.

4.- SIMULATION OF THE BIOSPHERE

The biosphere simulation is a simple module that, through multiplicative factors, converts the geosphere output values (mol/y) into dose values (Sv/y).

V.- REFERENCES

1.- Iman,R.L.; Shortencarier,M.J., "A FORTRAN 77 Program and User's Guide for Generation of Latin Hipercube and Random Samples for Use with Computer Models". NUREG/CR-3624. March, 1984.

2.- Pinedo,P., "Modelización del campo cercano de un almacenamiento de residuos radiactivos. Código VAULT-CTN". Julio 1989. CTN-81/89.

3.- Sherman,G.R., et al., "The System Variability Analisys Code SYVAC2 and Submodels for the second Interim Assessment of the Canadian Concept for Nuclear Fuel Disposal". TR-317. AECL, October 1986.

4.- Anders,D.A.,"Computational Fluid Mechanics and Heat Transfer". 1984 Mc Graw Hill.

5.- Hopkirk,R.J., "TROUGH-1D, Transport of Radioactive Outflows in Undergroun Hydrology (1 Dimension). User's Handbook and Theoretical Description". CH-8032 Zurich, 1987.

Participant: E Code: LISA-1A/JRC Organisation: CEC/Ispra

The LISA code has been adapted in order to run the level 1a exercise. In particular the waste form and vault submodels have been coded ex-novo for the purpose of the exercise. Two iterations of the test case have been made, to investigate the effect of different assumptions concerning the vault transport. The results discussed in section 3 of this report pertain to the second iteration.

FIRST ITERATION

Submodels description - WASTE FORM. According to the Level 1a specifications /1/ the nulcear waste is embedded into a matrix waste form within a steel canister. Canister failure is supposed to take place at a constant rate, all the canister beeing open at time=TDRUM. The concrete in each canister is also supposed to dissolve at constant rate, the entire amount being dissolved at time=TMATRX. TDRUM can either be smaller or greater than TMATRX, and both parameter are described by a distribution. The fraction of waste form dissolved at any given time t must then be computed by the convolution of the two processes. The coding is given in Appendix A.

Submodels description - VAULT. According to the test case specifications /1/ the following processes have been modelled within the vault:

* Advective transport

* Chemical retention, governed by a linear isotherm

* Element precipitation following solubility limits. because different isotopes of the same element are present in the input inventory, multiple isotope precipitation has to be accounted for.

* Chain decay, both in the solution-sorbed and precipitated phases (as well as within the waste matrix)

The vault submodel implemented in LISA takes advective transport into account (ie it is not a reaction tank model). The numerical scheme implemented is very simple, explicit of the first order, in both space and time, and will probably be upgraded if this module wii have to be used for more extended applications.

In order to take the multiple isotope precipitation into account the two actinide chains have been artificially merged into one. For each run the module analyses the decay chain and detects the number of isotopes for each element. Then, for each time step, the time derivative of concentration is computed.

Before integration the derivative is compared with that imposed by solubility, and the necessary adjustments are made.

The vault submodel has a built in mass balance check algorithm, which provides, for a number of specified times (TCHECK(I)), the balance of the nuclide between matrix, precipitate, sorbed, and solution phases. This is compared with the amount of nuclide which has already left the vault (adjusted for decay) and with the total inventory (adjusted for decay). A typical output is shown in Table 1 below

Table 1 Mass balance check in vault

```
BALANCE REQUESTED FOR T  =3.313E+02
PROVIDED FORT            =3.313E+02
CTOT. IN MATRIX          =0.000E+00
CTOT. SOLUT+SORBED       =3.703E+05
CTOT. PRECIPITATE        =1.101E+04
CTOT. OUTPUT             =3.903E+04
==================================
CTOTAL=4.204E+05
CTOT. MOLES IN VAULT (IF V=0) =4.204E+05
```

The example refers to the deterministic run number 1 and the check is made for the actinide chain (U238 plus Np237 chains). At the checking time tcheck=331 years all the waste form has dissolved, most of the actinide are in the sorbed state, and there is some precipitated uranium (mostly U238). The time consuming step in evaluating this mass balance is to compute the total output at time=tcheck; the output moles at each integration step must be scaled of the amount decayed up to time tcheck, and this must be done for all the TCHECK(I) time points.

The vault submodel also outputs the beginning and the end of the precipitation phase for each nuclide.

The total vault porosity (TPOVLT) has been used in order to compute geosphere retentions, although it might be argued that this implies diffusion into dead end porosities. Advective transport within the vault is governed by the vault interstitial velocity, computed from the darcy velocity and the effective porosity. The precipitation in the vault is computed assuming as vault volume the volume of the galleries (excluding the intact concrete between the galleries).

In order to be consistent with this assumption the flow in the vault has been computed as the product of the Darcy velocity and the effective (=galleries) cross section of the vault. This conflicts with the specification document, which suggest to use the total vault cross section. A choice has to be made here between the two

assumptions.The difference between the two is of about a factor two (see second iteration).

Submodels description - FAR FIELD. The TROUGH code was used for the Level1a intercomparison , with the same configuration used for the level E. Some work has been done in the direction of writing a new far field module, but due to the limited time available we are not yet ready to use it. The water flow through the geosphere has been computed as the product of the total vault cross section and the Darcy velocity in the first layer of the geosphere.Altough this seems a reasonable choice the specification document seems to indicate that there should not be any diluition before the end of the geosphere (see second iteration).

SECOND ITERATION

The following modifications have been made as a result of a first comparison with the results from other participants.

* The effective vault porosity has been used to compute retention in the vault. This corresponds to neglect completely diffusion in the vault.

* The total vault cross sectional area has been used in order to compute water flow in the vault; the advection term in the vault submodel had to be modified in order to be consistent with the new release rate.

* The water flow rate in the geosphere has been equated to that in the vault, in order to avoid diluition.

* An interpolation error has been detected in the algorithm to compute total doses at the time point for the deterministic runs. The error has been corrected.

Comments on the test case specification

Here is a list of problems encountered in the implementation of the exercise, ordered from the most to the least relevant.

*CPU time. Even when using the Crank Nickolson scheme implemented in TROUGH, which is implicitely stable, it is customary to have space and time steps discretised in such a way that the information does not travel more than a grid point in a time step. Furthermore, in order to take dispersion into proper account, it is advisable that space step does not exceed too much the dispersion length. Input data for the present intercomparison are highly unfavourable in this respect, as they couple very high path lenghts with very short dispersion length. For deterministic run number 1 the ratio LPATH1/LDISP1 is 90 and that LPATH2/LDISP2 is 340; in the most unfavourable situation these two figures can become 110 and 460. This implies a high number of space grid points, which coupled with the long release times imposed by the solubility limits lead to extremely time consuming computations. Even with a t=1 million year cut-off the exercise is too time

consuming.Furthermore, for the U238 chain, the short half life of Pb210 leads to very short time steps in my vault, which uses an explicit scheme.

*Input data. LISA had to be modified in order to accept the input distributions in the form suggested at the page 8 of the specification document /1/. May be Such a burden to the partecipants could be avoided by uniforming the input to the format used for Level E.

*Possible ambiguity. The test case let the user free to choice a proper use for the vault total and effective porosities. There is some inconsistency between the volume for precipitation in the vault and the use of the total vaultcross sectional area for the advective transport. In conclusion the scaling up of the difficulties between Level E and Level 1a appears adequate to objective of the exercise.

References

/1/ A. Nies, Level 1A case specification. GSF technical document, Braunschweig (D), October 1988

Appendix A
Coding of waste form submodel

```
DICTIONARY:

TONUDR=TOTAL NUMBER OF DRUMS
CONCR1=AMOUNT OF CONCRETE IN ONE DRUM (KG)
TDRUM=TIME FOR FAILURE OF LAST DRUM (A)
TMATRX=TIME FOR COMPLETE DEGRADATION OF THE CON-
CRETE IN ONE DRUM AFTER DRUM FAILURE (A)
TICODR=FAILURE RATE OF DRUM (=1/TDRUM, 1/A, CON-
STANT)
TICODR=DEGRADATION RATE OF CONCRETE (=1/TMATRX,
1/A, CONST)

DOCUMENTATION:

THE TWO CASES TDRUM>TMATRX AND TDRUM<TMATRX HAVE
BEEN CONSIDERED

CASE A.1: TMATRX<TDRUM AND T<TMATRX

FOR TMATRX < TDRUM THE AMOUNT OF CONCRETE DQ(T,T')
DISSOLVED UP TO TIME T DUE TO A CANISTER FAILURE
TAKING PLACE AT T' WHEN T<TMATRX IS
```

```
DQ(T,T')=TONUDR*TICODR*DT'*CONCR1*TICOMA*(T-T')(1
```

INTEGRATING ON T' EQ.1 BETWEEN ZERO AND T THE
TOTAL AMOUNT OF DISSOLVED CONTRETE AT TIME T IS

```
Q(T)=TONUDR*CONCR1*TICODR*TICOMA*T**2/2 (2
```

AND DERIVING THE ABOVE THE FLUX OF CONCRETE RESULTS

```
DQ(T)/DT=TONUDR*CONCR1*TICODR*TICOMA*T (3
```

For the other cases similar equations are derived
which are not described here.

```
DEBUG SUBCHK
END DEBUG
FUNCTION FLUXIN(TIME)
COMMON /CONST/TMAX,TOCC,CONCR1,TONUDR,
  &TSV,TMO,XVLT,DYGEO,
  &CSAVLT,TSAVLT,CONDEN,TPOVLT,DENGE1,
  &DENGE2,WING,TPOGE1,TPOGE2
COMMON /VAR/TMATRX,TDRUM,DCYVLT,VDCYL1,VDCYL2,
  &PORVLT,PORGE1,PORGE2,XPATH1,XPATH2,
  &CDIFF1,CDIFF2,XDISP1,XDISP2,FDILUT
COMMON /RUNCNT/NSTART,NRUN,NCHAIN,JOP
TICOMA=1./TMATRX
TICODR=1./TDRUM
CONST=TONUDR*CONCR1
T1=AMIN1(TMATRX,TDRUM)
T2=AMAX1(TMATRX,TDRUM)
IF(TIME.LT.0..OR.TIME.GT.(T1+T2)) THEN
  FLUXIN=0.
  RETURN
ELSEIF(TIME.LT.T1) THEN
  FLUXIN=CONST*TICODR*TICOMA*TIME
  RETURN
ELSEIF(TIME.GE.T1.AND.TIME.LT.T2) THEN
  FLUXIN=CONST/T2
  RETURN
ELSEIF(TIME.GE.T2.AND.TIME.LE.(T1+T2)) THEN
  FLUXIN=CONST*TICODR*(1.-TICOMA*(TIME-TDRUM))
  RETURN
ENDIF
END
```

Participant: F Code: MASCOT-3 Organisation: HARWELL/U.K.

Standard sub-models already available in MASCOT-3 were used throughout. However, as the following explains, some of these sub-models were applied in ways other than originally envisaged, so as to match as nearly as possible the requirements of the test case.

MASCOT-3 normally only delivers outputs from the final sub-model. Consequently, the deterministic cases were each run twice, with and without the geosphere and biosphere sub-models, so as to obtain both the vault behaviour results for questions C1 and C2, and the dose results for C3 and C4.

Vault: Models Used

The vault was modelled using 3 standard MASCOT-3 submodels:

- CONTAINMENT
- SOLUBILITY LIMITED SOURCE TERM
- STANDARD GEOSPHERE

The CONTAINMENT sub-model takes in the prescribed initial inventories, and can calculate decay and in-growth during a period of absolute containment. However, this period was set to zero for the Level-1a exercise.

The SOLUBILITY LIMITED SOURCE TERM sub-model in MASCOT-3 is based on the same conceptual model as used in the STRAW code, which is briefly described in the notes accompanying the submission to PSACOIN Level 1a using STRAW. The mathematical treatment in the MASCOT-3 sub-model is, however, simplified in such a way that the release rates of each radionuclide can be expressed analytically in the Laplace-transform domain. When any radionuclide is not solubility limited, its release rate is precisely the same as predicted by STRAW. When solubility limitation applies from the beginning, the initial release rates match those given by STRAW, but the subsequent time variation is different. The match is excellent when solubility limitation lasts for a long time; in other cases, the match is qualitative only, but the total predicted release agrees rather well.

There are never any 'corners' in the predicted release-rate vs. time functions corresponding to the ending of solubility limitation, so Question C2 can only be answered approximately. We have reported the period during which the concentration exceeds half the solubility limit. This is illustrated in Figure 1 attached.

The spread of drum failure and matrix degradation specified in the exercise were features which could not be directly modelled in MASCOT-3. The associated delays in release were simulated by a dummy STANDARD GEOSPHERE sub-model, placed AFTER the main source model. When the source model is behaving linearly, as it does when solubility limitation does not apply, then the correct solution of the differential equations in the STRAW model is obtained by convoluting the response from instantaneous release into solution with two 'top-hat' functions, representing drum-failure and matrix-degradation spread. With solubility limitation, the source behaviour is non-linear, and this approach is no longer correct, but it is the best available within the framework of MASCOT-3. In fact, MASCOT-3 does not even allow convolution with the two 'top-hat' functions, so we used a dummy STANDARD GEOSPHERE model instead, with parameters chosen to match the

first two moments of the desired delaying function. This is illustrated in Figure 2 attached.

Vault: Assumptions

In applying the above models to the Level 1a exercise, the following interpretations were applied to the specified data. The Darcy velocity used in calculating release rates was set to VDARCYL1*FDARCYVLT. The respository area, as used in calculating release rates by advection, was calculated using a cross-sectional area equal to 200m x 115m, as instructed on p.5 of the case specification. The repository volume was taken as 157500 cubic metres, i.e. the volume enclosed by the walls of the vault (excluding the intact rock between the galleries). These two assumptions are somewhat inconsistent, but these appeared to be the intentions of the case specification.

For the mass of repository materials participating in linear equilibrium sorption, non-cement constituents were ignored, and the effective density was obtained from Table 1 of the specification, as the quoted 'cement density', reduced according to the 'total porosity within the vault':

RHO = 2500 (1 - 0.20) kg per cubic metre.

The proportion of the repository volume occupied by porewater participating in the sorption partitioning was taken to be PORVLT. Had we used the 'total porosity' instead of PORVLT, the release rates of radionuclides not subject to solubility limitation would have been reduced by a factor of up to 2. While this could noticeably affect the comparison with other code results, we would not consider this uncertainty very significant in practice, considering the great uncertainties of experimental KD values.

Geosphere: Models

The POROUS GEOSPHERE sub-model of MASCOT-3 was used for each of the two geosphere layers. The equations solved for each layer are

$$Rn \frac{d\,Cn(x,t)}{d\,t} + v \frac{d\,Cn(x,t)}{d\,x} - D \frac{d2\,Cn(x,t)}{d\,x2} = LAMBDAp\ Rp\ Cp(x,t) - LAMBDAn\ Rn\ Cn(x,t) \qquad (1)$$

with initial conditions

$$Cn(x,0) = 0 \qquad (2)$$

and boundary conditions

$$PHI\ A\ v\ Cn(0,t) - PHI\ A\ D \frac{d\,Cn(0,t)}{d\,x} = Fn(t), \qquad (3)$$

$$Cn(L,t) = 0. \qquad (4)$$

In these equations, Cn(x,t) is the concentration of radionuclide n at position x and time t; Cp(x,t) is the same thing for a parent nuclide decaying to n. Rn is a retardation coefficient, v is mean porewater translation velocity, D is a dispersion coefficient, and LAMBDAp and LAMBDAn are decay constants for nuclides p and n.

Boundary condition (3) indicates that the total flux of nuclide n across x = 0 through area A of rock with effective porosity PHI is prescribed as Fn(t). Condition (4) indicates zero concentration at the end of the layer, x = L. Trials using condition (4) at x = infinity instead of x = L gave very similar results.

The outputs from the sub-model are the fluxes crossing x = L, evaluated as in (3).

The solution to equations (1) to (4) can be written down analytically after Laplace transformation of the time variable. MASCOT-3 uses these Laplace-domain solutions directly, with inversion to the time domain postponed until after the final sub-model.

Geosphere: Assumptions

In applying the above model to the Level 1a exercise, the following interpretations were applied to the specified data. The given Darcy velocity in layer x, VDARCYLx, was divided by the effective porosity PORLx, to give the flow velocity v in equations (1) and (3). The total dispersion coefficient was obtained as

$$D = v\ LDISPx + CDIFFx \qquad (5)$$

from the specified dispersion length LDISPx and effective diffusion coefficient CDIFFx for layer x.

The retardation factors were calculated as

$$Rn = 1 + RHO\ Kn\ /\ PORTOTx, \qquad (6)$$

where Kn are the sorption values given in Table 4 of the specification. RHO is the dry bulk density for the layer, obtained as

$$RHO = RHOSOLx\ (1 - PORTOTx), \qquad (7)$$

where RHOSOLx and PORTOTx are the rock density and total porosity values given in Table 1 for layer x.

The use of PORTOTx in equations (6) and (7), but PORLx to obtain v from the Darcy velocity, was in accordance with our understanding of the instructions on p.7 of the case specification. Normally we would use the flowing porosity, PORLx, on the denominator of (6), on the assumption that only the flowing porosity is filled with contaminated water and participates in the partitioning between dissolved and sorbed nuclides which the Kn factors characterise. On the other hand, we would also normally multiply experimental Kn values by an 'availability factor', representing the possibility that not all the rock mass is effectively available to participate in sorption to the extent that it is in the experimental setup. Thus, the use of PORTOTx in equation (6) is equivalent to making our 'availability factor' equal to (PORLx / PORTOTx).

The radionuclide fluxes out of the repository were used as inputs to layer1, and the fluxes out of layer 1 were used as inputs to layer 2. No dilution was applied at these interfaces. The values used for PHI and A in equation (3) are immaterial, since similar expressions are used for both the input and output fluxes for each layer.

Biosphere: Models and Assumptions

The MASCOT-3 sub-models STREAM DILUTION BIOSPHERE and DOSES were used. The first, designed for representing dilution in a stream or river, simply multiplies radionuclide release rates by a factor w/W, where w is an individual drinking water consumption rate, and W is the stream flow rate (both volume per year). The DOSES sub-model simply applies dose conversion factors (Sv/Bq) to obtain effective dose-rate contributions from each nuclide.

The use of drinking water consumption and dose conversion factors accords with the Level 1a case specification. These factors were to be applied to 'diluted concentration', calculated by applying the factor FDILUT to nominal concentrations at the end of layer 2, having neglected any change of flow rate between the source and the end of the geosphere. We took this 'diluted concentration' to be FDILUT, multiplied by our calculated molar flux out of layer 2 (mol/year), divided by the undiluted flow rate (cubic metres per year) of contaminated water, i.e. that through the source, given by the product of Darcy velocity within the repository, and the repository area. All of this was equivalent to setting our nominal stream flow rate to

$$W = FDARCYVLT\ VDARCYL1\ A\ /\ FDILUT, \qquad (8)$$

where A is the repository area.

FIGURE 1 PSACOIN LEVEL 1A: ILLUSTRATING DETERMINATION OF SOLUBILITY LIMIT PERIODS (Tc-99 IN DETRUN2)

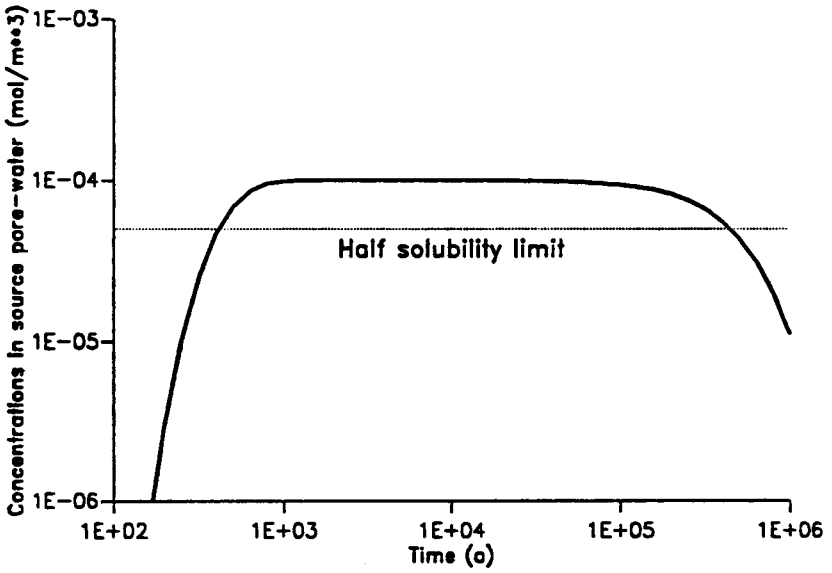
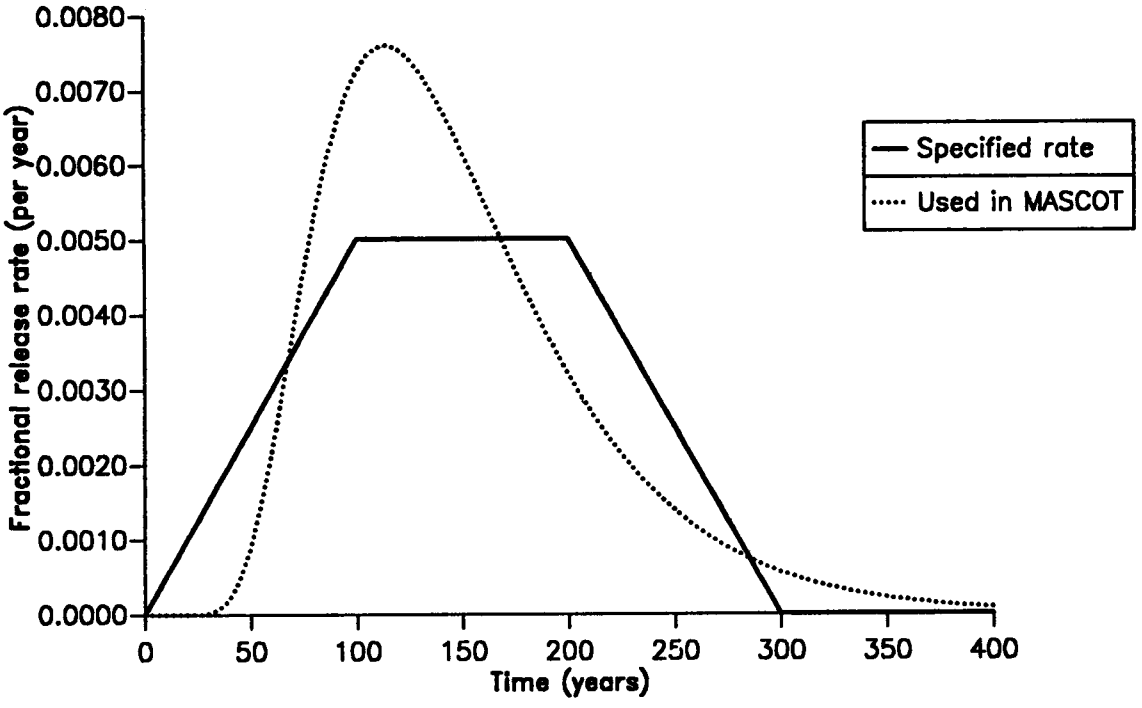


FIGURE 2 PSACOIN LEVEL 1A: SIMULATION IN MASCOT-3 OF DRUM FAILURE AND MATRIX DEGRADATION RATES



Participant: G Code: STRAW-1.1 Organisation: HARWELL, U.K.

STRAW is a deterministic research code, which models only the vault in any detail. It has no geosphere model, and only a simple dilution model of the biosphere, to obtain nominal drinking-water toxicity levels. Consequently, it is suitable for answering only questions C1 and C2 in the Level 1a exercise.

Model

After an assumed period of total containment (during which the radionuclides experience decay/in-growth within the cannisters), all radionuclides are assumed to immediately dissolve to a uniform concentration in the porewater within the repository, and to immediately establish linear sorption equilibrium with the cementitious materials. The concentration of each element in the porewater is subject to a specified solubility limit. Whenever this limit applies, the proportion in solution of each isotope of an element is taken to be the same as the proportion in the total current inventory. Transport of the dissolved radionuclides out of the repository is assumed to be purely advective, so that the release rate of each is calculated as the product of the concentration in the pore water, the Darcy velocity of the porewater flow within the repository, and the cross-sectional area of the repository normal to the flow.

The calculation centres around solution of the differential equations

$$\frac{d\,Mij(t)}{d\,t} = -\,LAMBDAij\;Mij(t) + LAMBDAIJ\;MIJ(t) - q\;A\;Cij(t) \qquad (1)$$

where, for isotope j of element i, Mij(t) is the molar inventory at time t, LAMBDAij is the decay constant, and Cij(t) is the concentration dissolved in the porewater. LAMBDAIJ and MIJ(t) are the decay constant and inventory of the parent radionuclide (if any). q is the Darcy velocity of the porewater flow, and A is the cross-sectional area. The concentrations Cij(t) are given by

$$Cij(t) = \begin{cases} 0 & : \; t < Tc \\ MIN\left(Mij(t) / ALPHAi\;V,\; CSi\;Mij(t) / MTOTi(t) \right) & : \; t > Tc \end{cases} \qquad (2)$$

where Tc is the containment time, CSi is the solubility limit for element i, MTOTi(t) is the sum over Mik(t) for all isotopes, k, of element i, V is the volume of the repository, while the capacity factors ALPHAi are given by

$$ALPHAi = PHI + BETA\;RHO\;Ki, \qquad (3)$$

where PHI is the proportion of the repository volume occupied by porewater, BETA is the fraction of the repository mass participating in the sorption, RHO is the mean density of the repository materials, and Ki is the sorption distribution coefficient for element i.

Equations (1) to (3) are solved numerically using Gear's method.

Assumptions

In applying the above model to the deterministic cases of PSACOIN Level 1a, q was set to the product VDARCYL1*FDARCYVLT. A was taken as the gross area of the repository, 200m * 115m, as instructed on p.5 of the case specification. V was taken as the volume enclosed by the walls of the vault (excluding the intact rock between the galleries). The assumptions for A and V seem to be somewhat inconsistent, but these appeared to be the intentions of the case specification.

STRAW could not model the spread of the cannister failure times and matrix degradation, so the containment time Tc was set to

Tc = (TDRUM + TMATRIX) / 2,

representing the mean delay in release of radionuclides into solution. This explains the zero results at 100 years in question C1. Similarly, when solubility limitation is indicated in question C2, the beginning times always equal Tc.

PHI was identified with PORVLT, BETA was set to unity, while RHO was obtained from Table 1 of the specification, as the quoted 'cement density', reduced according to the 'total porosity within the vault':

RHO = 2500 (1 - 0.20) kg per cubic metre.

The meaning in the specification of 'effective porosity in the vault', PORVLT, was not entirely clear. Had we used the 'total porosity' instead of PORVLT for our PHI, the release rates of radionuclides not subject to solubility limitation would have been reduced by a factor of up to 2. While this could noticeably affect the comparison with other code results, we would not consider this uncertainty very significant in practice, considering the great uncertainties of experimental values for the sorption coefficients Ki, and of the appropriate value for the availability factor BETA.

Participant: H Code: SYVAC/FI Organisation: VTT/Finland

1. Introduction

In this note, we will discuss mainly conceptual modelling of the near-field and dilution because they most remarkably affect the results obtained. For geosphere migration modelling the original SYVAC A/C submodel with some modifications related to time-stepping has been employed.

The numerical results required in the Level 1a questionnaire have been sent to the NEA Data Bank via the computer network. Additional results are presented as figures in the Appendix.

The reader of this note is assumed to be familiar with the PSACOIN Level 1a case specification [1].

2. Near-field modelling

A special near-field model was developed for the PSACOIN Level 1a exercise. The release of radionuclides out of the vault has been assumed to take place **by convection** with the groundwater flow through the vault **and by diffusion** through the walls of vault. The inside of the vault has been modelled as a **homogeneous mixing tank**. (Fig. 1).

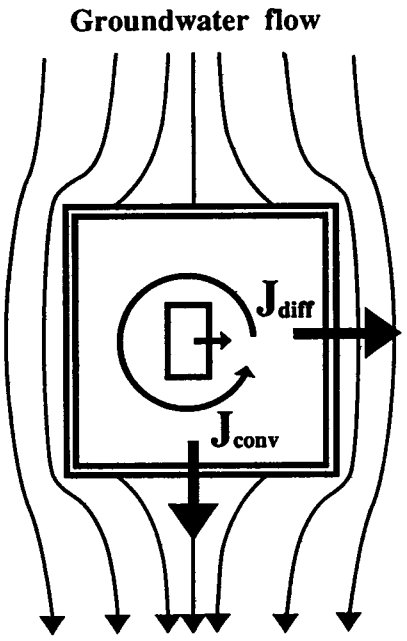


Fig. 1. Conceptual modelling of the near-field.

In presenting the modelling ideas, the following notations are used:

$a_i(t)$ is the total amount of the nuclide i as a funtion of time (mol)
$s_i(t)$ is the release rate out of the waste packages (mol/a),
$b_i(t)$ is the amount of the nuclide in the vault outside of the packages (mol),
$c_{i,w}(t)$ is the concentration in the vault water phase (mol/m^3),
$J_i(t)$ is the release rate out of the vault (mol/a).

The total amount of the nuclide i obeys the following equation:

$$\dot{a}_i(t) = \lambda_{i-1} a_{i-1}(t) - \lambda_i a_i(t). \qquad (1)$$

The release rate out of the packages was derived to be:

$$s_i(t) = \frac{a_i(t)}{TMATRIX \cdot TDRUM} \cdot [\min(t,TDRUM) - \max(0,(t-TMATRIX))],$$

$$t \leq TDRUM + TMATRIX$$

$$s_i(t) = 0 \qquad t > TDRUM + TMATRIX \qquad (2)$$

The balance equation for the amount of a nuclide in the vault outside of the packages is

$$\dot{b}_i(t) = s_i(t) - J_{i,conv}(t) - J_{i,diff}(t) + \lambda_{i-1} b_{i-1}(t) - \lambda_i b_i(t) \qquad (3)$$

where $J_{i,conv}(t)$ and $J_{i,diff}(t)$ are release rates out of the vault by convection and diffusion, respectively.

The concentration of a nuclide in the water phase of the vault is:

$$c_{i,w}(t) = \min [(b_i(t)/(R_i \cdot V_b(t) \cdot \varepsilon_b), (b_i(t)/\Sigma b_{n,i}(t)) \cdot c_{sol})]. \qquad (4)$$

In deriving of the solubility limit for a particular nuclide, the potential existence of other nuclides of the same element ($b_{n,i}$'s) in the vault is accounted for. In the following, the subscript i is dropped off to simplify the expressions. The retardation factor of a nuclide in the buffer material is:

$$R = 1 + [(1-\varepsilon_b)/\varepsilon_b] \cdot K_{Db} \cdot \rho_{s,b}. \qquad (5)$$

The sorbent material in the vault consist of the buffer material outside of the packages and of the matrix material of the failured waste packages. The sorbent volume is hence a funtion of time:

$$V_b(t) = V_{bo} + (t/TDRUM)\cdot V_{bp} \quad , t \leq TDRUM$$

$$V_b(t) = V_{bo} + V_{bp} \quad , t > TDRUM \qquad (6)$$

where

V_{bo} is the volume of sorbing material in the vault outside of the packages (m^3),
V_{bp} is the total volume of sorbing material in the waste packages (m^3).

The release rate of a nuclide out of the vault by convection with the groundwater flow through the vault is:

$$J_{conv}(t) = FDARCY\cdot VDARCY1\cdot A_b\cdot c_w(t) \qquad (7)$$

where

A_b is the area of the bottom of the vault (m^2).

The release rate of a nuclide out the vault by diffusion is affected 1) by the mass transfer through the buffer material layer between the waste packages and the rock and 2) by the mass transfer resistance caused by the fact that the nuclides must be transferred from the stagnant water in the vault into groundwater flowing in the rock around the vault. When FDARCY > 1, there is no diffusive release out of the vault, because all groundwater flowing in the close vicinity of the vault is directed through the vault and will accordingly leave the vault with the same nuclide concentration as the water in the vault. The diffusive release rate was hence modelled to be:

$$J_{diff}(t) = (r_1\cdot r_2)/(r_1+r_2)\cdot c_w(t), \quad FDARCY \leq 1$$

$$J_{diff}(t) = 0 \quad FDARCY > 1 \qquad (8)$$

where

$$r_1 = D_w\cdot G\cdot \varepsilon_b\cdot[2\cdot(1-FDARCY)\cdot A_b + A_w] / d_w \qquad (9)$$

and

$$r_2 = [2\cdot(1-FDARCY)\cdot A_b + A_w)]\cdot PORL1\cdot \qquad (10)$$

$$\{(4\cdot D_w\cdot VDARCY1/PORL1) / [\ \pi\cdot((1-FDARCY)\cdot l_1 + l_2)\}^{1/2}$$

where

D_w is the molecular diffusion coefficient in water (m^2/a),
G is the geometrical factor for diffusion in the buffer material,
ε_b is the porosity of the buffer material,
A_b is the area of the bottom of the vault (m^2),
A_w is the area of the side walls of the vault (m^2),

d_w is the thickness of the buffer material layer between the outermost waste packages and the rock (m),
l_1 is the width of a tunnel of the the vault (m),
l_2 is the heigth of the vault (m), and
VDARCY1 is the Darcy velocity in the layer 1 (m/a),
FDARCY is the ratio of Darcy velocity in the vault to that in the layer 1,
PORL1 is the effective porosity in the layer 1.

The equation (9) represents the diffusion mass transfer coefficient through a wall with a thickness of d_w and with a zero-outside-concentration boundary condition. The factor (1-FDARCY) takes into account the fact that the area for diffusion release is reduced by increased FDARCY. The equation (10) represents the diffusion mass transfer coefficient from a stagnant water phase into the flowing groundwater around the vault. The derivation of the equation is presented in ref. [2 and 3]. Also here, the factor (1-FDARCY) takes into account the reducing of the interface area and pathlength when FDARCY is increased.

The total release rate out of the vault is simply:

$$J(t) = J_{conv}(t) + J_{diff}(t). \qquad (11)$$

3. Modelling of dilution

We consider dilution modelling for the Level 1a case somewhat tricky, because the case specification can, in our mind, be interpreted in different ways. The interpretation applied by us is the following: Nuclides released from the vault into the geosphere are assumed to be mixed in the groundwater flowing through the area occupied of the vault, and the dilution factor FDILUT specifies then the dilution taking place in the geosphere and at the geosphere-biosphere interface. The dose rate due to a nuclide can hence be expressed as:

$$h(t) = \frac{FDILUT \cdot e(t) \cdot w \cdot d_c}{VDARCY1 \cdot A_{vault}} \qquad (12)$$

where

e(t) is the undiluted release rate from the geosphere into the biosphere (Bq/a),
w is the intake of water by man (m^3/a),
d_c is the dose conversion factor (Sv/Bq),
VDARCY1 is the Darcy velocity in layer 1 (m/a),
A_{vault} is the cross-sectional rock area occupied by the vault (m^2).

It should be noted, that the "primary" dilution volume specified in the above equation as $VDARCY1 \cdot A_{vault}$ is not equal to the groundwater flow through the vault ($FDARCY \cdot VDARCY1 \cdot A_b$).

4. Data

The above equations include parameters for which values were not directly given in the case specification. The following data values have been used:

V_{bo} volume of the buffer material around waste packages in the vault and in the bottom of the vault: 35000 m^3,
V_{bp} volume of matrix material in the waste packages: 108000 m^3,
A_b area of the bottom of the vault: 10500 m^2,
A_w area of the side walls of the vault: 20000 m^2,
l_1 width of the tunnels of the vault: 15 m,
l_2 heigth of the vault: 15 m,
d_w thickness of the buffer material layer between the outermost waste packages and the rock: 0.5 m,
D_w molecular diffusion coefficient in water: $6.3 \cdot 10^{-2}$ m^2/a,
G geometrical factor for diffusion in the buffer material: 10^{-2},
A_{vault} cross-section area of the vault: 23000 m^2.

With the parameter range given in the case specification, the following ranges can be derived for some key measures:

- groundwater flow through the vault: 0.105...210 m^3/a,
- amount of groundwater in which the nuclides released out of the vault are mixed: 23...230 m^3/a,
- $J_{conv}(t)$ = [0.105...210 m^3/a]$\cdot c_w(t)$,
- $J_{diff}(t)$ = [3.4...8.9 m^3/a] $\cdot c_w(t)$, FDARCY $\leq$ 1
- $J_{diff}(t)$ = 0 , FDARCY > 1.

With the values specified for the three determistic runs, the following intermediate results are obtained:

		DETRUN1	DETRUN2	DETRUN3
$J_{conv}(t)$	[$m^3/a \cdot c_w(t)$]	210	0.1	8.2
$J_{diff}(t)$	[$m^3/a \cdot c_w(t)$]	0	6.9	7.8
$J_{tot}(t)$	[$m^3/a \cdot c_w(t)$]	210	7.0	16.0
Prim. dilution vol. [m^3/a]		230	23.0	126.5
Concentration of nuclides released out of the vault	[$\cdot c_w(t)$]	0.91	0.30	0.13

In the above expressions $c_w(t)$ is the concentration of a nuclide in the water phase of the vault as a function of time.

References

1. Nies, A., PSACOIN - Level 1a Case Specification. Final Draft (October 1988).
2. Neretnieks, I., Transport of oxidants and radionuclides through a clay barrier. KBS Teknisk Rapport 79, 1978.
3. Karlsson, L.-G., et al., Nuclide release from the near-field of a L/ILW repository. NAGRA, Technical Report 85-33, 1985.

Participant: I Code: VANDAL-1.2C Organisation: DOE/U.K.

The fundamental concept upon which VANDAL is based is a network analogy in which the flow and transport pathways in the geosphere are approximated by a network of streamtubes. VANDAL first solves the groundwater flow network using Darcy's model. The obtained velocities are then used in the advective diffusive transport through the network. Nuclide flow rates are collected at bioreceptor(s) to calculate dose-to-man using the multi-composer time? biosphere submodel. Finally, the source can be embedded in any path of the network (Reference [1]).

Since the principle objective of Level 1a) is to measure the bias between various modelling approaches, no transformation to the code was done to match the specification.

1. Groundwater Velocities

Since groundwater velocities are not a direct input of VANDAL, it has been necessary to set a network that will accept the constraints of the specifications. The following network was used:

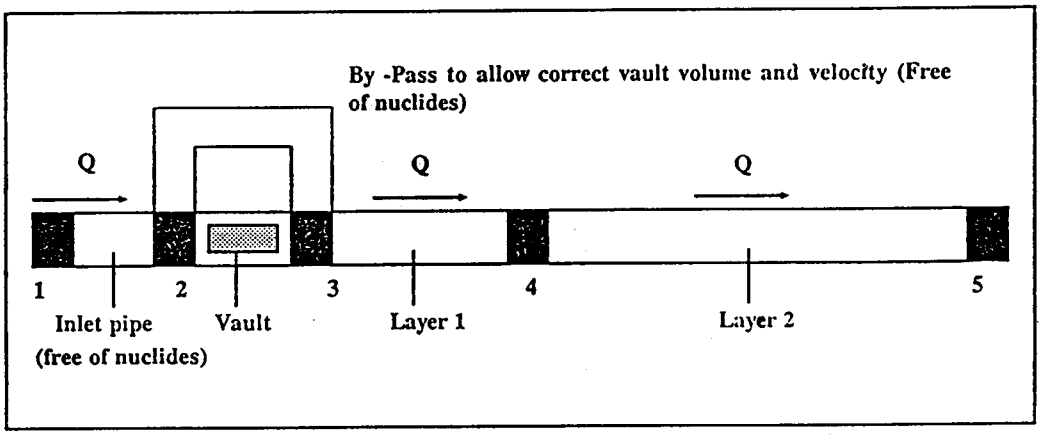


Figure 1. VANDAL Network used for the Level 1a) exercise

The flow Q is the same for Layer 1 and 2 as required by the specifications. The cross-section areas of the layers are adjusted to match the specified velocities as:

cross-section area = flow/velocity

The flow itself is imposed in the specification by:

Q = FDARCTVLT x Velocity (Layer 1) x Vault Cross-Section Area

The inclusion of a by-pass was necessary to respect the dimensions of the result as well as the specified ratio of velocities.

Finally, to avoid the effects of lengths variation on velocities, the ratio: length/hydraulic conductivity, is kept constant for the two layers. The distribution of parameters used in VANDAL were derived as described above from the original specified parameters. To verify that the original distributions are respected, preliminary runs of the flow calculation were performed using the derived distributions.

2. Near-Field Modelling

To conform to the principal objective of Level 1a), no alteration were made to the near-field model of VANDAL although the release process is imposed in the specification.

The deposition of TMATRIX is not applicable in VANDAL. The life time of the canisters, TDRUM, was set using an appropriate corrosion rate. The solubility limit in VANDAL only applies in release from drums. The argument to use such a model is that in a realistic situation the highest concentration if found in the drums and that many case precipitation leads to heavier particles which cannot be transported using the standard method. The release from drums occurs by two processes: leaching and wash-out. The leaching process is diffusive whilst the wash-out is a purely advective transport. For these reasons it is expected that:

a) VANDAL will produce a faster release than a code like EMOS.

b) The period of exceeding solubility limits (Table C2 of the questionnaire) is not an appropriate question for VANDAL.

3. Geosphere Model

The transport through the two layers is modelled using the standard one-dimensional advective/diffusive transport equation.

A numerical finite difference method is used to solve the equations. The code works in terms of concentration and the boundary conditions are reset at the end of each timestep. Independent tests of layer 2 discretisation showed that representing this layer with one path of the network was acceptable. The concentrations are calculated as a function of the volume of water. There is therefore an implicit dilution occurring within the layers.

Finally, with the exception of the parameters involved in the flow calculation, the parameters used for the geosphere are the same as the specifications. The kinetic porosity is used to calculate the average pore velocity and the resultant dispersion coefficient. The total porosity is used to calculate the retardation factor and the effective diffusion coefficient. It is also important to note that K_d are not sampled are independent variables.

4. Biosphere Model

The biosphere simulation conforms to the specification. The dilution factor includes a correction term for the dilution that already occurred in the geosphere transport.

[1] J-M Laurens, B.G.J. Thompson and T. Sumerling. The development and application of an integrated radiological risk assessment procedure using time-dependent probabilistic risk analysis. International Symposium on the Safety Assessment of Radioactive Waste Repositories, Paris 9-13 October 1989. (Paper 50).

Participant: J Code: (E)LISA-01 Organisation: CIEMAT/Spain

The LISA code has been used for PSACOIN Level 1A, and two different iterations were made. For the first, the case was run using the LISA version adapted to the Level 1A specifications (Saltelli, 1989) and implemented on CIEMAT's computer system (VAX-785). Relatively insignificant modifications were incorporated into the original version, all of them related to the different type of computer (from AMDAHL-470/V8 to VAX-785). In the second iteration, significant changes were made to the LISA code, consisting of a new geosphere module (GTM-01), a different way of dealing with the isotopes in the vault in order to optimise the problem solubility, and other minor improvements throughout the program.

SUBMODEL DESCRIPTIONS

WASTE FORM

According to the Level 1A specifications, the nuclear wastes are embedded in a cement matrix contained within a steel canister. Both barriers are described by their respective lifetimes. A constant rate for the canister failure is considered between the beginning of the post-operational phase and the time when the last container loses its integrity (TDRUM). The degradation of concrete in each canister also follows a constant rate (congruent dissolution), starting its dissolution after the failure of the canister, complete dissolution taking place at time TMATRIX. TDRUM can either be smaller or greater than TMATRIX, and both of them are described by a probability distribution function. The net release from the waste form is computed by integral convolution of the two processes.

VAULT

According to the Level 1A specifications, the following processes are to be modelled within the vault:

- advective transport,
- chemical retention, governed by a linear isotherm,
- element precipitation following solubility limits (because different isotopes of the same element can be present in the input inventory, multiple isotope precipitation has to be accounted for), and
- radioactive decay (both in dissolved and precipitated phases, as well as within the waste matrix).

The specifications for a given geometry of the vault are included. The advective transport equation in LISA for the vault module is approximated by the finite-difference method. The equation includes advective transport, chemical retention, and radioactive decay:

$$R \frac{dC}{dt} = -V \frac{dC}{dX} - \lambda R C + \lambda^{\circ} R^{\circ} C^{\circ} ,$$

where R is the nuclide-dependent retardation coefficient, C is the concentration (i.e., the amount transported per unit time), t is the time, V is the groundwater interstitial velocity, X is the space or length coordinate, λ is the nuclide-dependent decay constant, and the superscript (°) indicates the parent nuclide.

The numerical scheme implemented is explicit to the first order in both space and time. Only one space node is considered for the backfill barrier (0.5 m). The precipitation-solution processes are evaluated for different times within each run and for all isotopes of a nuclide present in the different decay chains considered (multiple isotope precipitation). To do that, and only for the vault submodel, chain decay with common isotopes of one nuclide are linked (Cuñado, 1989). The initial inventory, the increase of it from the parent decay, and the decay of each isotope are considered independently. In this way, it is not necessary to use a dummy nuclide to merge artificially the two chains. For each time step, the time derivative of concentration is computed. Before integration, the derivative is compared with that imposed by solubility, and the necessary adjustments are made. The vault submodel has a built-in mass-balance-check algorithm, which provides, for a number of specified times, the balance of nuclides between matrix, precipitate, sorbed, and solution phases. This is compared with the amount of nuclides which have already left the vault (adjusted for decay) and with the total inventory (adjusted for decay).

The effective vault porosity has been used to compute retention in the vault. Advective transport within the vault is governed by the vault interstitial velocity (V), computed from the Darcy velocity (V_d) and the effective porosity (m_e):

$$V_r = \frac{V_d}{m_e} = \frac{V_d * A_t}{m_t * A_r}$$

where m_t is the total porosity, A_t is the total vault area, and A_r is the real vault area.

Precipitation in the vault is computed assuming as vault volume the volume of the galleries (excluding the intact concrete between the galleries). The flow in the vault has been computed as the product of the Darcy velocity and the effective area of the vault (A_r). This conflicts with the specifications, which instead suggest the total vault cross-sectional area (A_t).

GEOSPHERE

A new geosphere module, GTM-01 (Geosphere Transport Model Release One), has been designed to replace the TROUGH-1D code formerly used in LISA. The framework of this development was a contract between ENRESA and JRC/Ispra. The

new code (Prado, 1989) was presented during the 9th Meeting of the PSAC User Group (Albuquerque, 1989). The processes considered by GTM are somewhat simpler than those of TROUGH. The main characteristic of the new module is that it is completely coded in FORTRAN-77 following the estructurated programming method, with good documentation and many comments in the listing. An attempt has been made to create a module that could be easily customised for use in different PSA codes. GTM solves the one-dimensional groundwater transport equation considering diffusion, dispersion, advection, retention, and decay:

$$R \frac{dC}{dt} = D \frac{d^2C}{dX^2} - V \frac{dC}{dX} - \lambda R C + \lambda^\circ R^\circ C^\circ$$

where D is the hydrodynamic dispersion coefficient, equal to $D^\circ + V\alpha$, D° is the geosphere dispersion coefficient, α is the geosphere diffusion coefficient, and the other variables are as defined above.

Decay chains of any number of elements and multilayered geosphere media are considered. The numerical scheme is the Crank-Nicolson implicit method. Two different analytical solutions are included in the code for user testing. The code has been verified by direct comparison against these analytical solutions and against the PSACOIN Level E benchmark results. The results obtained by GTM-01 show good agreement both with the Level E results and with the analytical solutions.

This module was incorporated into LISA-1A (Ruiz and Francia, 1989), to replace the TROUGH code. Good agreement is shown between the results of the second iteration and those obtained by other benchmark participants in the first iteration.

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Prado, P., 1989. ENRESA/JRC Cooperation Agreement in the Field of Nuclear Waste Management. Final Report (Chapter 3: GTM-01 Geosphere Tranpsort Model Release 1). CEC/JRC, Ispra.

Ruiz, C. and Francia, L., 1989. LISA-1A Code Listing Program. First Version with GTM-01 Submodule for the Geosphere. CIEMAT-ITN, Madrid.

Saltelli, A., 1989. LISA Code for PSACOIN Level-1a Exercise. Listing Program. CEC/JRC, Ispra.

Participant: K Code: NEFTRAN-B.2 Organisation: SNL/U.S.A.

The NEFTRAN (NEtwork Flow and TRANsport) computer code was developed by Sandia National Laboratories for performance assessment calculations for high-level radioactive waste repositories. NEFTRAN uses the analytic solution of the convective-dispersion equation for particle density (concentration) in one dimension for each leg in a connected flow network.

Unlike the finite difference and finite element techniques, the NEFTRAN analytical technique needs a high (1.5 and above) Courant number (velocity * time-step / spatial grid length). If the Courant number is too low (below 1.0), then numerical dispersion can occur with NEFTRAN. With NEFTRAN, the Courant number is bounded from below by maximum acceptable numerical dispersion and from above by the desired time resolution of the results. For the PSAC problem here, the desired time resolution of the source term was the critical factor in determining the Courant number (and the time step), which sometimes was low enough to cause numerical dispersion. A fine spatial mesh was used to increase the Courant number to more acceptable levels. In effect, the small time step required to resolve the PSAC source term release was the determining factor in choosing NEFTRAN's time step, and this negated NEFTRAN's capability of using large time steps, which has always been one of its unique features.

Some assumptions were made for required parameter values that were not specified in the PSACOIN Level 1a case specification. The leg length for the source (vault) was taken to be 1.1 m, which is the length of the canister. The leg length for the bottom half of the vault below the canister was taken to be 6.95 m. The total thickness of the vault was given as 15 m with the canisters of length 1.1 m and located in the middle of the vault (6.95 + 1.1 + 6.95 = 15.).

A relatively small dispersivity value of 0.0001 m (less than one thousandth of the source leg of 1.1 m) was chosen to model the dispersion in the vault (for both the source leg and the bottom vault leg). This dispersivity was not specified in the PSACOIN Level 1a specification.

The third and fourth legs in NEFTRAN correspond to the first and second legs in the PSACOIN Level 1a specification. NEFTRAN requires a discharge area of the last leg for concentration calculations. Since this area was not specified in the Level 1a specification, we calculated the value by equating the Darcy fluxes (Darcy velocity times area) of the fourth (last) leg and the vault, and then solving for the discharge area. In other words,

AREA = FDARCYVLT * VDARCYL1 * 23,000. / VDARCYL2

where FDARCYVLT * VDARCYL1 is the Darcy velocity in the vault (both vault legs), 23,000 is the cross-sectional area (m^2) of the vault, and VDARCYL2 is the Darcy velocity in the fourth leg (the third and last migration leg).

Because of the relatively short release periods of the source, a small time step (25 to 100 years) was required to resolve the release rate curve. This small step could not be changed for later time periods after the total release of the source. As a result, the run times of NEFTRAN were around 20 minutes on a VAX 8650 (about 4 times faster than a VAX 780) for 100,000 years of simulation. Since the run times were large, we did not vary the Kd values in the stochastic case, since this would have required about another 50 runs (10 radionuclides for each leg times the number of legs times 3/2) using the Latin Hypercube Sampling technique; Iman and Helton (1985) have given the rule of thumb for the number of realizations required to be greater than 4/3 (conservatively taken to be 3/2) times the number of parameters. We kept, for the stochastic case, the Kd values fixed at their values used for DETRUN3 (Deterministic Run 3). Hence, the standard deviations of the NEFTRAN results should be smaller than other results obtained by also varying the Kd values.

The solubility limits were not part of the NEFTRAN model, and were not used at all except for comparison with calculated concentrations. The radionuclide concentrations were calculated at the beginning of the second vault leg where they are the highest except for the source leg itself (the first leg). These concentrations were then compared to the solubility limits given for each of the three deterministic runs.

REFERENCES

Iman, R.L., and J.C. Helton, 1985. A Comparison of Uncertainty and Sensitivity Analysis Techniques for Computer Models, SAND84-1461 (NUREG/CR-3904). Sandia National Laboratories, Albuquerque, NM.

Participant: L Code: SYVAC3-L1A Organisation: AECL/Canada

The starting point for SYVAC3-L1A was SYVAC3-CC3, which is being used to assess the Canadian concept for nuclear fuel waste disposal. The SYVAC3 executive part of the code was used without change. The model code is discussed in detail below.

Executive Code

The number and sizes of time steps are set by a time series management package in the SYVAC3 executive to achieve a requested "target fraction error" for the representation of a function as a time series. The fractional error of the representation is calculated by comparing estimates of the area bounded by the function. The time steps are variable, with more times used in regions where they are required to follow the shape of the function being represented. With this type of time step control, greatest accuracy is achieved near the peaks of a function and lesser accuracy is tolerated where the function has smaller values far from the peaks. To get accurate values far from the peak values, the user can specify a set of fixed times which will appear in every time series. The target fractional error is then applied between each pair of adjacent fixed times.

The deterministic runs have a target fractional error of 0.001 with fixed times at 100, 1000, 4000, 5000, 10000, 50000, 100000, 500000, and 1000000 years. A maximum number of 200 time points in the 1000000 year time frame was used, with time steps varying in length from less than one year to 500000 years. The probabilistic case has a target fractional error of 0.05, with fixed times at 5000, 10000, 50000, 100000, 500000, and 1000000 years. A maximum number of 100 time points in the 1000000 year time frame was used, with time steps varying in length from less than one year to 500000 years.

Transport calculations are done using an analytical solution to the one-dimensional convection-dispersion-retardation-decay chain mass-balance differential-equation (CDE). This analytical response-function is numerically convoluted with a numerical time series representation of the flux of nuclides at the inlet to the transport region. These convolutions are performed by SYVAC3 utility routines from the time series management package.

Vault

The CC3 vault model was completely replaced by new code for the PSAC Level 1A problem. The new code uses the same building blocks as the CC3 model such as release from the waste form, convolution with container failure rate, precipitation, and transport across the buffer/backfill.

For the Level 1A problem, the vault is modelled as a continuously distributed source. The release from a single container is spatially convoluted, using the response-function for the CDE with semi-infinite outlet boundary condition, over the region of the vault where containers are placed to give the total nuclide flow to the level of the vault floor. Retardation factors for the nuclides in the cement are calculated using the total porosity within the vault given in Table 1 and not the sampled value for PORVLT in Table 3.

Solubility constraints are applied nuclide by nuclide and account is not taken of the simultaneous presence of three different isotopes of Uranium. The given (or sampled) value for the solubility limit for an element is used for each isotope in turn. This approximation will have little affect on the U^{238} results. However, the other isotopes of Uranium will be less likely to reach a solubility constraint and may be released from the vault at higher concentrations than if coprecipitation with the U^{238} were accounted for. Solubility limitations are applied at the vault floor level, using the area of the vault galleries: 10,500 square metres. The maximum flow rate from the vault floor, SLIMRR, for each nuclide is determined from:

SLIMRR = FDARCYVLT * VDARCYL1 * AREAUN * SOLUNX

where SOLUNX is the solubility limit for the corresponding element given in Table 4, and AREAUN is 10,500 square metres.

A previous iteration of these calculations used the total vault area: 23,000 square metres, for this solubility calculation. The larger value for area gives 2.2 times more flow out of the vault for nuclides that have reached their solubility limit over what is obtained in the current results. However, using the gallery area in the current results gives an implied dilution by a factor of 2.2 as the flow enters layer 1 of the geosphere. This is an ambiguous point in the specifications.

Transport of the solubility limited flow of nuclides through the 0.50 metre cement floor of the vault is done using the response-function for the CDE with semi-infinite outlet boundary condition. Again, retardation factors for the nuclides in the cement are calculated using the total porosity within the vault given in Table 1 not the value for PORVLT in Table 3.

Dispersion length in the vault is set to zero. However diffusion constants cannot also be zero in our model and are set to 1.0E-04 square metres per year, about an order of magnitude below the normal physical values.

Geosphere

The CC3 geosphere model was used without substantive change. A module was added to convert the PSAC sampled parameters into the parameters required by the model, (e.g. darcy velocity to linear velocity). The geosphere is modelled as a two segment system, using the response-function for the CDE with semi-infinite outlet boundary condition in each segment. The mass flow passing through segment one at the required distance (90 to 110 m) from the inlet is used as input to segment two. The mass flow through segment two at the required distance (17 to 23 Km) from the inlet is used as input to the well. The control of the number of segments and their connectivity and geometry is done through the input file and no code changes are needed.

The factor FDILUT is used to determine the dilution of nuclides in the water coming from the well. To calculate the nuclide concentration in the well water, the nuclide flow rate from the geosphere transport calculation is divided by the total water flow rate, QWDEM, given by:

QWDEM = VDARCY1 * FDARCYVLT * TVAREA / FDILUT,

where TVAREA is the total vault area of 23,000 square metres. However, as described above, the use of the gallery area of 10,500 m^2 for the solubility calculation implies an additional dilution by a factor of 2.2 upon entering layer 1 of the geosphere for nuclides that have reached their solubility limit.

The effective diffusion constants in layers 1 and 2 were interpreted, in the absence of an explicit definition, as excluding a porosity factor. (In a previous iteration of the calculations it was assumed a porosity factor was included in the effective diffusion constant). The dispersion coefficient, D1, for layer 1 was calculated from:

D1 = LDISP1*VDARCYL1/PORL1 + CDIFF1

with a similar expression for layer 2.

Biosphere

The CC3 biosphere model was used without any coding change, and included all its pathways. In general, we find that the drinking water pathway produces small doses when compared to other ingestion pathways. However, for the Level 1A problems, zero parameter values were introduced into the model where necessary to make the final dose calculation include only the well-drinking water pathway.

Comments on Results Obtained

In Table 3.1, our final dose result for U^{234} in DETRUN3 occurs at significantly longer time, 400000 years, than the bulk of the other participants, 100000 to 130000 years.

We have adopted a spatially distributed source in the vault with a spatial convolution done to collect nuclides at the level of the floor of the vault. This concept yields a nuclide flow rate to the floor of the vault that reaches an approximately a constant value over a long time period. This type of behaviour is reasonable and to be expected from this concept of the vault. See solid curves on Figures 1 and 2 for U^{238} and U^{234} results. Solubility constraints are applied at the vault floor level, but we do not have U^{234} reaching a solubility limit, partly because of the low amounts reaching the vault floor and partly because we have ignored coprecipitation with U^{238}. At times greater than 100000 years there is a slight increase in the amount of U^{234} flowing from the vault into the 0.5 m vault floor due to ingrowth from the large amount of U^{238} precipitated at this point.

In contrast, a mixing tank approach has all input to the mixing tank in the first few hundred years, (TDRUM + TMATRIX), thus giving larger amounts at early times. Release from a mixing tank is proportional to the inventory in the mixing tank with release rate falling at a rate due to the residence time/mixing properties of the hypothetical tank. The largest releases are at early times. Hence the peak in the dose curve occurs shortly after breakthrough and at higher levels.

The near constant rates of nuclide flow that we obtained for both U^{238} and U^{234} are propagated, with additional delay, through the 0.5 m vault floor and through the two geosphere layers. See the other curves on Figures 1 and 2. Hence, the final dose curves for U^{238} and U^{234} are nearly constant after breakthrough to the biosphere is reached in about 100000 years. See Figure 3 for final dose curves from the U^{238} chain. The slight rise of the U^{234} curve formally puts its maximum at near 400000 years. This rise and maximum are more clearly evident in the linear scale plot on Figure 4. However, breakthrough of U^{234} is complete by 100000 years and our results are not inconsistent with the times of maximum reported in the 100000 to 130000 year range. Hence, we believe our results for U^{234} in DETRUN3 are correct and accurately represent the scenario being modelled.

Regardless of the retarding effect of the cement placed around the containers themselves, the 0.50 metre thick cement floor is a significant barrier to transport of all the nuclides and, in particular, prevents any early releases from the vault of nuclides that are sorbed by the cement. For example in DETRUN3, the water transit time through this barrier alone is 97 years and the retarded transit time for Uranium is over 12000 years (see Figures 1 and 2). This observation is at odds with the results reported by some participants in Table C1, and explains why we report no release of Uranium at the 100 year and 1000 year time points. Similar conclusions hold for many of the other nuclides and for DETRUN2 and DETRUN1.

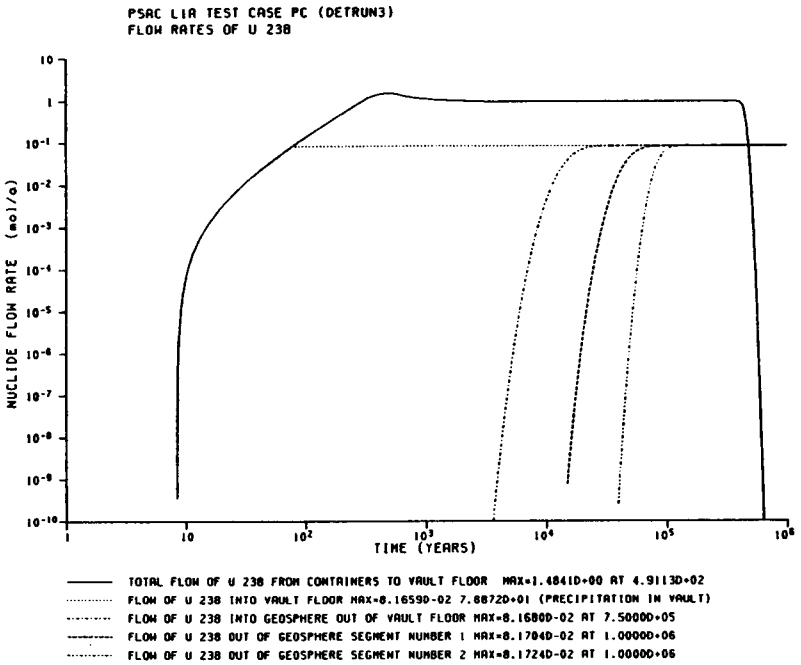

FIGURE 1

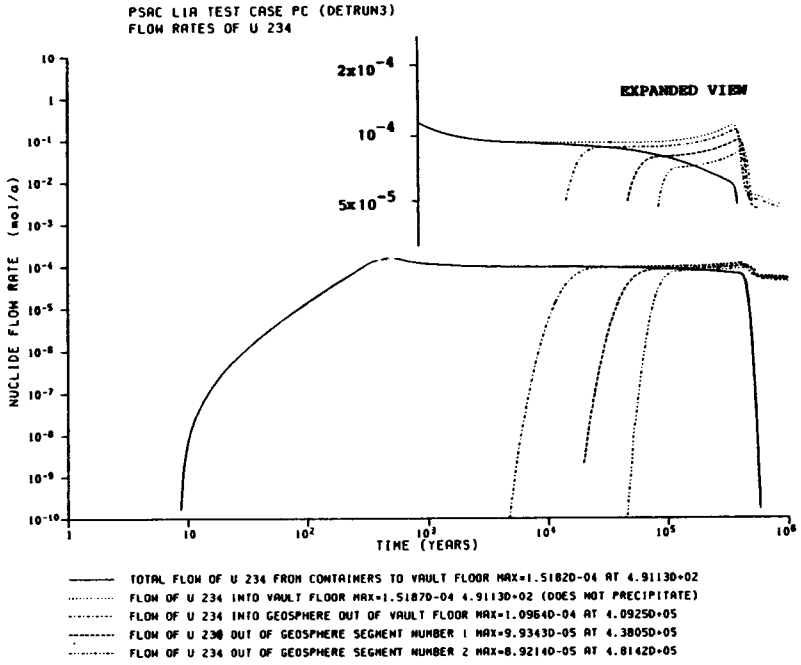

FIGURE 2

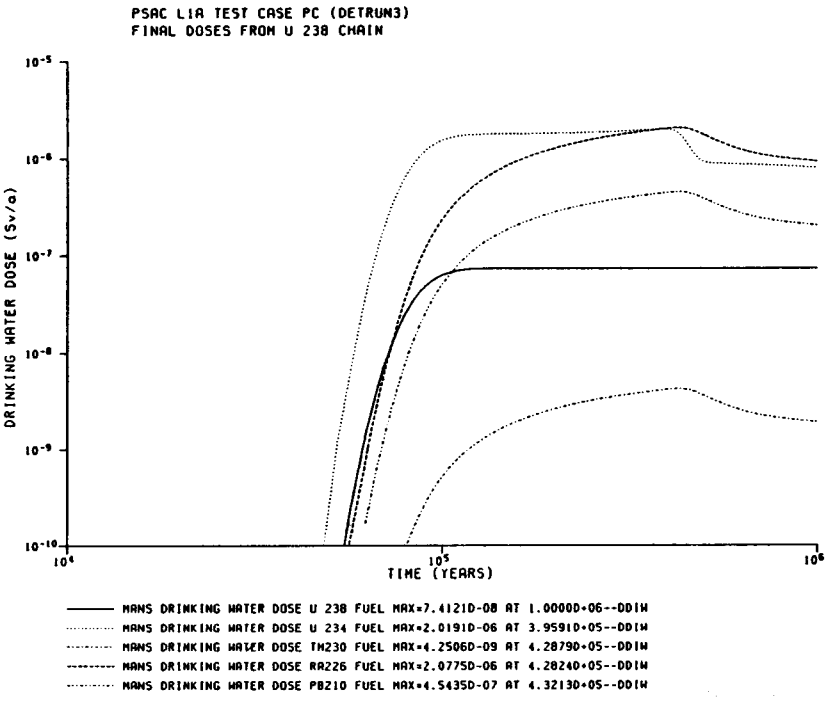

FIGURE 3

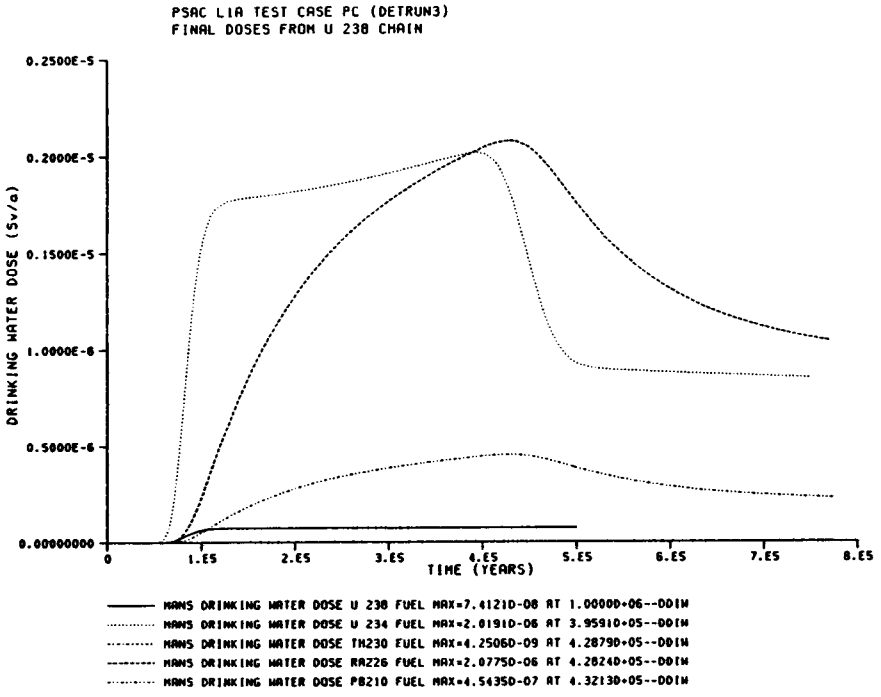

FIGURE 4

ANNEX C

Tables of Original Results from Case Studies

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

These data are provided here in order that readers may perform further analyses of the contributed data, should they so wish. All of the results submitted by participants are also freely available in machine-readable form from the NEA Data Bank.

DETRUN1-3 RELEASE RATES TC-99 (TABLE C1 OF QUESTIONNAIRE)

	DETRUN1			DETRUN 2			DETRUN 3	
	100	1000	100	1000	1000000	100	1000	10000 a
A EMOS4	1.1E+00	7.3E-05	7.8E-06	2.3E-05	1.0E-05	7.5E-03	1.2E-01	9.4E-03
B JAERI-1.4	1.1E+00	1.2E-04	8.4E-06	2.3E-05	8.9E-06	7.9E-03	1.2E-01	8.8E-03
C LISA-1A/CI	1.0E+00	4.1E-05	3.5E-06	1.1E-05	4.8E-06	4.5E-03	7.8E-02	1.7E-02
D SIMPAR-2.0	2.5E+00	0.	1.1E-14	6.1E-07	5.4E-06	7.2E-05	9.1E-02	1.2E-03
E LISA-1A/JRC	1.2E+00	2.1E-06	9.1E-06	2.3E-05	8.3E-06	8.4E-03	1.3E-01	1.9E-03
F MASCOT-3	1.8E+00	1.9E-06	1.1E-09	2.3E-05	2.6E-06	5.9E-04	1.3E-01	6.8E-03
G STRAW-1.1	N.C.	1.3E-08	N.C.	2.3E-05	9.6E-06	N.C.	1.3E-01	6.9E-03
H SYVAC/FI	6.6E-01	1.2E-02	7.0E-04	7.0E-04	2.6E-11	1.5E-02	1.1E-01	9.0E-03
I VANDAL-1.2C	3.4E-01	8.0E-02	0.	4.3E-07	2.0E-06	1.1E-03	8.2E-02	9.4E-03
J (E)LISA-01	1.2E+00	2.1E-06	9.1E-06	2.3E-05	8.3E-06	8.4E-03	1.2E-01	7.2E-03
K NEFTRAN-B.2	2.0E+00	0.	0.	0.	0.	0.	0.	8.9E-09
L SYVAC3-L1A	7.4E-01	0.	0.	2.4E-09	8.6E-06	1.3E-08	7.1E-02	2.4E-07

DETRUN1-3 RELEASE RATES I-129 (TABLE C1 OF QUESTIONNAIRE)

	DETRUN1			DETRUN 2			DETRUN 3	
	100	1000	100	1000	1000000	100	1000	10000 a
A EMOS4	1.8E+00	3.5E-05	1.3E-04	5.6E-03	2.6E-06	2.3E-02	3.0E-01	1.7E-03
B JAERI-1.4	1.8E+00	7.0E-05	1.4E-04	5.6E-03	3.7E-06	2.4E-02	3.0E-01	1.8E-03
C LISA-1A/CI	1.7E+00	1.2E-05	5.9E-05	2.6E-03	8.7E-05	1.4E-02	2.1E-01	9.9E-03
D SIMPAR-2.0	4.0E+00	0.	2.2E-11	1.2E-04	2.4E-12	7.8E-04	3.1E-01	3.7E-10
E LISA-1A/JRC	1.9E+00	5.4E-07	1.5E-04	5.6E-03	2.8E-06	2.6E-02	3.6E-01	1.4E-06
F MASCOT-3	3.1E+00	1.8E-06	2.8E-07	5.6E-03	3.7E-06	2.1E-03	3.5E-01	3.8E-04
G STRAW-1.1	N.C.	3.7E-10	N.C.	5.5E-03	3.6E-06	N.C.	3.4E-01	3.7E-04
H SYVAC/FI	1.1E+00	1.2E-02	1.2E-02	1.7E-01	0.	4.6E-02	2.9E-01	1.9E-03
I VANDAL-1.2C	2.0E+00	1.1E-08	0.	6.4E-04	4.7E-06	8.5E-03	1.9E-01	5.2E-04
J (E)LISA-01	1.9E+00	5.4E-07	1.5E-04	5.6E-03	2.8E-06	2.5E-02	3.0E-01	7.2E-04
K NEFTRAN-B.2	3.0E+00	0.	0.	0.	0.	0.	0.	<1.0E-22
L SYVAC3-L1A	1.2E+00	0.	4.5E-08	4.6E-03	3.2E-06	9.8E-05	2.1E-01	0.

DETRUN1-3 RELEASE RATES NP-237 (TABLE C1 OF QUESTIONNAIRE)

	DETRUN1			DETRUN 2			DETRUN 3	
	100	1000	100	1000	1000000	100	1000	10000 a
A EMOS4	1.4E-02	4.8E-02	7.2E-09	2.3E-07	2.2E-07	1.3E-05	2.4E-04	2.4E-04
B JAERI-1.4	1.5E-02	4.7E-02	7.7E-09	2.3E-07	2.2E-07	1.3E-05	2.4E-04	2.4E-04
C LISA-1A/CI	1.3E-02	4.5E-02	3.2E-09	1.1E-07	1.0E-07	7.6E-06	1.5E-04	1.4E-04
D SIMPAR-2.0	5.3E-03	9.4E-02	0.	1.3E-12	1.7E-09	2.2E-12	2.4E-06	3.0E-05
E LISA-1A/JRC	1.5E-02	4.7E-02	8.4E-09	2.3E-07	2.2E-07	1.4E-05	2.4E-04	2.4E-04
F MASCOT-3	1.4E-02	4.8E-02	1.1E-11	2.3E-07	2.2E-07	8.6E-07	2.4E-04	2.4E-04
G STRAW-1.1	N.C.	4.9E-02	N.C.	2.3E-07	2.3E-07	N.C.	2.4E-04	2.4E-04
H SYVAC/FI	7.5E-03	2.7E-02	6.5E-07	7.0E-06	7.0E-06	2.6E-05	2.3E-04	2.3E-04
I VANDAL-1.2C	3.7E-03	3.0E-02	0.	6.2E-11	2.0E-08	6.8E-09	1.8E-06	2.0E-05
J (E)LISA-01	1.5E-02	4.7E-02	8.4E-09	2.3E-07	2.2E-07	1.4E-05	2.4E-04	2.4E-04
K NEFTRAN-B.2	0.	0.	0.	0.	3.8E-14	0.	0.	0.
L SYVAC3-L1A	0.	2.9E-02	0.	0.	1.1E-09	0.	0.	9.0E-19

DETRUN1-3 RELEASE RATES U-238 (TABLE C1 OF QUESTIONNAIRE)

	DETRUN1			DETRUN 2			DETRUN 3	
	100	1000	100	1000	1000000	100	1000	10000 a
A EMOS4	1.3E+02	1.9E+02	2.3E-05	2.3E-05	2.3E-05	1.3E-01	1.8E-01	1.8E-01
B JAERI-1.4	1.3E+02	1.8E+02	2.3E-05	2.3E-05	2.3E-05	1.3E-01	1.8E-01	1.8E-01
C LISA-1A/CI	1.2E+02	1.9E+02	1.1E-05	1.1E-05	1.0E-05	7.5E-02	1.1E-01	1.1E-01
D SIMPAR-2.0	1.6E+02	3.5E+02	0.	8.5E-09	1.1E-05	5.3E-07	8.8E-02	7.5E-01
E LISA-1A/JRC	1.4E+02	1.8E+02	2.3E-05	2.3E-05	2.3E-05	1.4E-01	1.8E-01	1.8E-01
F MASCOT-3	1.0E+02	2.1E+02	1.1E-09	2.3E-05	2.3E-05	6.4E-04	1.8E-01	1.8E-01
G STRAW-1.1	N.C.	1.8E+02	N.C.	2.3E-05	2.3E-05	N.C.	1.8E-01	1.8E-01
H SYVAC/FI	6.8E+01	1.6E+02	6.7E-04	7.0E-04	7.0E-04	1.5E-01	1.6E-01	1.6E-01
I VANDAL-1.2C	9.8E+02	8.1E+01	0.	2.3E-08	2.7E-06	3.1E-05	4.5E-03	3.5E-02
J (E)LISA-01	1.4E+02	1.8E+02	2.3E-05	2.3E-05	2.3E-05	1.4E-01	1.8E-01	1.8E-01
K NEFTRAN-B.2	0.	2.2E-02	0.	0.	2.0E-08	0.	0.	0.
L SYVAC3-L1A	1.3E+01	2.1E+02	0.	0.	3.1E-06	0.	0.	1.7E-02

DETRUN1-3 RELEASE RATES U-234 (TABLE C1 OF QUESTIONNAIRE)

	DETRUN1			DETRUN 2			DETRUN 3	
	100	1000	100	1000	1000000	100	1000	10000 a
A EMOS4	1.3E-02	1.9E-02	2.3E-09	2.3E-09	1.3E-09	1.3E-05	1.8E-05	1.8E-05
B JAERI-1.4	1.3E-02	1.8E-02	2.3E-09	2.3E-09	1.3E-09	1.3E-05	1.8E-05	1.7E-05
C LISA-1A/CI	1.2E-02	2.0E-02	1.1E-09	1.1E-09	6.3E-09	7.6E-06	9.1E-05	1.4E-04
D SIMPAR-2.0	1.7E-02	3.5E-02	0.	8.6E-13	6.1E-10	5.4E-11	8.9E-06	7.6E-05
E LISA-1A/JRC	1.4E-02	1.8E-02	2.3E-09	2.4E-09	2.7E-09	1.4E-05	1.8E-05	1.8E-05
F MASCOT-3	1.0E-02	1.9E-02	1.1E-13	2.3E-09	1.3E-09	6.5E-08	1.8E-05	1.8E-05
G STRAW-1.1	N.C.	1.9E-02	N.C.	2.4E-09	1.3E-09	N.C.	1.9E-05	1.8E-05
H SYVAC/FI	6.9E-03	1.6E-02	6.8E-08	7.1E-08	4.0E-08	1.5E-05	1.6E-05	1.6E-05
I VANDAL-1.2C	1.3E-02	7.9E-03	0.	5.3E-10	1.9E-08	6.8E-08	9.3E-06	5.5E-05
J (E)LISA-01	1.4E-02	1.8E-02	2.3E-09	2.3E-09	1.3E-09	1.4E-05	1.8E-05	1.8E-05
K NEFTRAN-B.2	0.	2.2E-06	0.	0.	6.4E-14	0.	0.	0.
L SYVAC3-L1A	1.4E-03	2.8E-02	0.	0.	1.4E-07	0.	0.	2.5E-05

DETRUN1-3 PERIODS EXCEEDING SOLUBILITY LIMITS TC-99 (TABLE C2 OF QUESTIONNAIRE)

	DETRUN 1		DETRUN 2		DETRUN 3	
A EMOS4	-	-	1.7E+02	7.3E+05	-	-
B JAERI-1.4	-	-	1.7E+02	7.6E+05	-	-
C LISA-1A/CI	-	-	1.6E+02	7.8E+05	-	-
D SIMPAR-2.0	-	-	3.7E+02	4.4E+02	-	-
E LISA-1A/JRC	-	-	1.6E+02	8.0E+05	-	-
F MASCOT-3	-	-	4.2E+02	4.5E+05	3.0E+02	2.1E+03
G STRAW-1.1	-	-	4.5E+02	7.8E+05	-	-
H SYVAC/FI	-	-	1.0E+02	3.2E+05	-	-
I VANDAL-1.2C	-	-	1.0E+03	1.0E+06	-	-
J (E)LISA-01	-	-	1.6E+02	7.6E+05	-	-
K NEFTRAN-B.2	-	-	5.0E+01	1.6E+05	-	-
L SYVAC3-L1A	-	-	1.1E+01	>1.0E+06	-	-

DETRUN1-3 PERIODS EXCEEDING SOLUBILITY LIMITS NP-237 (TABLE C2 OF QUESTIONNAIRE)

	DETRUN 1		DETRUN 2		DETRUN 3	
A EMOS4	-	-	5.8E+02	8.6E+05	-	-
B JAERI-1.4	-	-	5.8E+02	8.8E+05	-	-
C LISA-1A/CI	-	-	5.9E+02	8.8E+05	-	-
D SIMPAR-2.0	-	-	-	-	-	-
E LISA-1A/JRC	-	-	5.9E+02	8.8E+05	-	-
F MASCOT-3	-	-	4.2E+02	>1.0E+06	-	-
G STRAW-1.1	-	-	4.5E+02	9.6E+05	-	-
H SYVAC/FI	-	-	5.6E+02	>1.0E+06	-	-
I VANDAL-1.2C	-	-	3.3E+02	1.0E+06	-	-
J (E)LISA-01	-	-	5.9E+02	8.8E+05	-	-
K NEFTRAN-B.2	-	-	5.0E+01	2.3E+05	1.3E+02	1.4E+03
L SYVAC3-L1A	-	-	3.0E+02	>1.0E+06	-	-

DETRUN1-3 PERIODS EXCEEDING SOLUBILITY LIMITS U-238 (TABLE C2 OF QUESTIONNAIRE)

	DETRUN 1		DETRUN 2		DETRUN 3	
A EMOS4	2.6E+02	3.0E+02	5.6E+01	>1.0E+06	1.2E+02	>1.0E+06
B JAERI-1.4	2.6E+02	3.0E+02	5.5E+01	>1.0E+06	1.2E+02	>1.0E+06
C LISA-1A/CI	2.5E+02	3.2E+02	5.4E+01	>1.0E+06	1.1E+02	>1.0E+06
D SIMPAR-2.0	-	-	6.0E+01	5.2E+02	2.3E+02	3.3E+02
E LISA-1A/JRC	2.2E+02	4.9E+02	5.4E+01	>1.0E+06	1.1E+02	>1.0E+06
F MASCOT-3	1.4E+02	9.1E+02	4.2E+02	>1.0E+06	2.8E+02	>1.0E+06
G STRAW-1.1	1.5E+02	3.4E+02	4.5E+02	>1.0E+06	3.0E+02	>1.0E+06
H SYVAC/FI	2.2E+02	5.6E+02	2.8E+01	>1.0E+06	8.0E+01	>1.0E+06
I VANDAL-1.2C	-	-	1.0E+05	1.0E+06	1.0E+03	1.0E+06
J (E)LISA-01	2.6E+02	3.0E+02	5.4E+01	>1.0E+06	1.1E+02	>1.0E+06
K NEFTRAN-B.2	-	-	5.0E+01	3.1E+05	1.3E+02	1.9E+03
L SYVAC3-L1A	2.1E+02	2.1E+03	5.6E+01	>1.0E+06	6.9E+01	>1.0E+06

DETRUN1-3 PEAK DOSE RATE AND TIME OF PEAK TC-99 (TABLE C3 OF QUESTIONNAIRE)

	DETRUN 1		DETRUN 2		DETRUN 3	
A EMOS4	2.5E-05	4.8E+03	3.7E-11	1.0E+06	3.9E-06	3.1E+04
B JAERI-1.4	2.5E-05	4.8E+03	3.6E-11	1.0E+06	3.9E-06	3.0E+04
C LISA-1A/CI	3.3E-05	4.8E+03	1.3E-13	9.8E+05	4.7E-07	3.6E+04
D SIMPAR-2.0	1.2E-05	1.3E+03	2.8E-09	5.1E+05	1.5E-06	9.3E+03
E LISA-1A/JRC	2.5E-05	4.8E+03	5.5E-11	1.0E+06	3.6E-06	3.0E+04
F MASCOT-3	2.6E-05	4.7E+03	5.0E-11	1.0E+06	4.2E-06	2.9E+04
G STRAW-1.1	N.C.	N.C.	N.C.	N.C.	N.C.	N.C.
H SYVAC/FI	2.3E-05	4.7E+03	1.1E-11	1.0E+06	5.7E-07	3.0E+04
I VANDAL-1.2C	4.0E-06	5.5E+03	1.9E-12	1.0E+06	4.7E-07	3.2E+04
J (E)LISA-01	2.5E-05	4.9E+03	2.8E-11	1.0E+06	3.7E-06	3.3E+04
K NEFTRAN-B.2	2.7E-05	4.8E+03	0.	1.0E+06	5.2E-06	3.1E+04
L SYVAC3-L1A	2.6E-05	4.8E+03	1.0E-11	1.0E+06	4.3E-06	3.2E+04

DETRUN1-3 PEAK DOSE RATE AND TIME OF PEAK I-129 (TABLE C3 OF QUESTIONNAIRE)

	DETRUN 1		DETRUN 2		DETRUN 3	
A EMOS4	1.0E-04	4.1E+03	8.7E-06	9.2E+04	3.9E-05	1.1E+04
B JAERI-1.4	1.0E-04	4.0E+03	8.6E-06	9.2E+04	3.9E-05	1.1E+04
C LISA-1A/CI	1.4E-04	4.1E+03	4.5E-08	1.0E+05	4.4E-06	1.2E+04
D SIMPAR-2.0	4.3E-05	1.1E+03	7.3E-07	1.1E+05	9.8E-06	5.1E+03
E LISA-1A/JRC	1.0E-04	4.0E+03	8.6E-06	8.7E+04	3.8E-05	1.1E+04
F MASCOT-3	1.1E-04	4.0E+03	8.7E-06	8.9E+04	4.4E-05	1.0E+04
G STRAW-1.1	N.C.	N.C.	N.C.	N.C.	N.C.	N.C.
H SYVAC/FI	9.8E-05	4.0E+03	4.5E-07	6.7E+04	5.6E-06	1.1E+04
I VANDAL-1.2C	2.5E-05	3.8E+03	4.5E-07	1.6E+05	5.3E-06	1.1E+04
J (E)LISA-01	1.0E-04	4.1E+03	8.6E-06	9.5E+04	3.7E-05	1.1E+04
K NEFTRAN-B.2	1.1E-04	4.0E+03	2.8E-05	2.2E+05	5.8E-05	1.1E+04
L SYVAC3-L1A	1.1E-04	4.0E+03	6.9E-06	8.9E+04	4.2E-05	1.2E+04

DETRUN1-3 PEAK DOSE RATE AND TIME OF PEAK NP-237 (TABLE C3 OF QUESTIONNAIRE)

	DETRUN 1		DETRUN 2		DETRUN 3	
A EMOS4	3.9E-04	2.0E+04	0.	1.0E+06	5.4E-06	4.9E+05
B JAERI-1.4	4.2E-04	2.0E+04	0.	1.0E+06	5.5E-06	4.9E+05
C LISA-1A/CI	6.1E-04	2.3E+04	0.	1.0E+06	4.8E-07	5.0E+05
D SIMPAR-2.0	1.1E-04	4.3E+03	0.	1.0E+06	6.0E-07	2.7E+05
E LISA-1A/JRC	3.8E-04	2.0E+04	0.	1.0E+06	5.3E-06	4.9E+05
F MASCOT-3	3.9E-04	2.0E+04	0.	1.0E+06	5.4E-06	4.8E+05
G STRAW-1.1	N.C.	N.C.	N.C.	N.C.	N.C.	N.C.
H SYVAC/FI	4.8E-04	2.0E+04	0.	1.0E+06	7.3E-07	5.0E+05
I VANDAL-1.2C	1.0E-04	2.4E+04	1.4E-15	1.0E+06	3.8E-07	9.1E+05
J (E)LISA-01	3.9E-04	2.1E+04	0.	1.0E+06	5.2E-06	5.1E+05
K NEFTRAN-B.2	8.1E-04	2.1E+04	0.	1.0E+06	5.2E-06	1.0E+06
L SYVAC3-L1A	3.5E-04	2.3E+04	0.	1.0E+06	9.9E-07	4.7E+05

DETRUN1-3 PEAK DOSE RATE AND TIME OF PEAK U-238 (TABLE C3 OF QUESTIONNAIRE)

	DETRUN 1		DETRUN 2		DETRUN 3	
A EMOS4	8.7E-05	6.8E+03	0.	1.0E+06	1.6E-07	6.2E+05
B JAERI-1.4	7.1E-05	6.8E+03	0.	1.0E+06	1.6E-07	1.7E+05
C LISA-1A/CI	1.3E-04	7.3E+03	0.	1.0E+06	1.4E-08	9.8E+05
D SIMPAR-2.0	3.2E-05	1.6E+03	1.9E-12	1.0E+06	1.4E-07	6.6E+04
E LISA-1A/JRC	8.4E-05	6.7E+03	0.	1.0E+06	1.6E-07	1.0E+06
F MASCOT-3	9.1E-05	6.8E+03	0.	1.0E+06	1.6E-07	1.3E+05
G STRAW-1.1	N.C.	N.C.	N.C.	N.C.	N.C.	N.C.
H SYVAC/FI	1.4E-04	6.7E+03	0.	1.0E+06	2.1E-08	4.7E+05
I VANDAL-1.2C	2.5E-05	7.3E+03	2.3E-15	1.0E+06	1.2E-07	6.9E+05
J (E)LISA-01	8.6E-05	6.8E+03	0.	1.0E+06	1.6E-07	1.0E+06
K NEFTRAN-B.2	1.5E-04	6.7E+03	0.	1.0E+06	7.2E-06	2.2E+05
L SYVAC3-L1A	7.3E-05	7.4E+03	0.	1.0E+06	7.4E-08	1.0E+06

DETRUN1-3 PEAK DOSE RATE AND TIME OF PEAK U-234 (TABLE C3 OF QUESTIONNAIRE)

	DETRUN 1		DETRUN 2		DETRUN 3	
A EMOS4	1.8E-04	6.8E+03	0.	1.0E+06	3.0E-07	1.1E+05
B JAERI-1.4	1.5E-04	6.8E+03	0.	1.0E+06	2.6E-07	1.0E+05
C LISA-1A/CI	2.8E-04	7.3E+03	0.	1.0E+06	2.8E-07	1.1E+05
D SIMPAR-2.0	6.7E-05	1.6E+03	2.1E-12	1.0E+06	2.8E-07	5.1E+04
E LISA-1A/JRC	1.8E-04	6.8E+03	0.	1.0E+06	3.0E-07	1.1E+05
F MASCOT-3	1.7E-04	6.8E+03	0.	1.0E+06	2.9E-07	1.1E+05
G STRAW-1.1	N.C.	N.C.	N.C.	N.C.	N.C.	N.C.
H SYVAC/FI	3.0E-04	6.7E+03	0.	1.0E+06	3.8E-08	1.1E+05
I VANDAL-1.2C	5.2E-05	7.3E+03	4.2E-14	1.0E+06	2.2E-07	1.8E+05
J (E)LISA-01	1.8E-04	6.8E+03	0.	1.0E+06	2.9E-07	1.3E+05
K NEFTRAN-B.2	3.0E-04	6.7E+03	0.	1.0E+06	1.2E-05	2.2E+05
L SYVAC3-L1A	1.9E-04	7.2E+03	0.	1.0E+06	2.0E-06	4.0E+05

DETRUN1 TOTAL DOSE RATES AT SELECTED TIMES (TABLE C4 OF QUESTIONNAIRE)

	4000	10000	100000	1000000 a
A EMOS4	1.1E-04	2.0E-05	3.8E-06	1.5E-09
B JAERI-1.4	1.1E-04	1.3E-05	6.8E-14	0.
C LISA-1A/CI	1.2E-05	6.6E-05	N.C.	N.C.
D SIMPAR-2.0	8.8E-05	2.1E-06	3.3E-07	0.
E LISA-1A/JRC	1.1E-04	1.5E-05	2.6E-06	9.6E-10
F MASCOT-3	1.1E-04	2.3E-05	3.7E-06	1.4E-09
G STRAW-1.1	N.C.	N.C.	N.C.	N.C.
H SYVAC/FI	1.0E-04	8.5E-05	8.2E-06	3.0E-09
I VANDAL-1.2C	2.6E-05	1.0E-04	2.3E-11	0.
J (E)LISA-01	1.0E-04	1.7E-05	2.7E-06	1.0E-09
K NEFTRAN-B.2	1.2E-04	8.6E-06	4.1E-06	0.
L SYVAC3-L1A	1.1E-04	1.4E-05	3.7E-06	1.4E-09

DETRUN2 TOTAL DOSE RATES AT SELECTED TIMES (TABLE C4 OF QUESTIONNAIRE)

	4000	10000	100000	1000000 a
A EMOS4	0.	0.	8.5E-06	8.4E-09
B JAERI-1.4	0.	0.	8.5E-06	1.2E-08
C LISA-1A/CI	0.	0.	4.4E-08	2.1E-09
D SIMPAR-2.0	0.	1.4E-11	6.9E-07	7.8E-10
E LISA-1A/JRC	0.	0.	8.3E-06	8.4E-09
F MASCOT-3	0.	0.	8.4E-06	1.2E-08
G STRAW-1.1	N.C.	N.C.	N.C.	N.C.
H SYVAC/FI	0.	0.	5.2E-08	1.1E-11
I VANDAL-1.2C	0.	0.	3.5E-07	2.6E-09
J (E)LISA-01	0.	0.	8.5E-06	9.5E-09
K NEFTRAN-B.2	0.	0.	0.	0.
L SYVAC3-L1A	0.	0.	6.7E-06	1.1E-08

DETRUN3 TOTAL DOSE RATES AT SELECTED TIMES (TABLE C4 OF QUESTIONNAIRE)

	4000	10000	100000	1000000 a
A EMOS4	9.3E-11	3.5E-05	6.7E-07	3.6E-06
B JAERI-1.4	9.8E-15	3.5E-05	4.5E-07	3.4E-06
C LISA-1A/CI	0.	1.4E-06	3.4E-07	5.3E-07
D SIMPAR-2.0	6.2E-06	2.8E-06	9.5E-07	5.1E-07
E LISA-1A/JRC	4.2E-11	3.3E-05	8.4E-07	3.7E-06
F MASCOT-3	0.	4.3E-05	6.9E-07	3.4E-06
G STRAW-1.1	N.C.	N.C.	N.C.	N.C.
H SYVAC/FI	6.0E-13	5.4E-06	8.7E-08	4.9E-07
I VANDAL-1.2C	2.1E-09	5.0E-06	3.1E-07	6.1E-07
J (E)LISA-01	1.7E-11	2.9E-05	7.1E-07	3.8E-06
K NEFTRAN-B.2	0.	3.9E-05	8.0E-11	6.7E-06
L SYVAC3-L1A	1.5E-15	2.8E-05	2.0E-06	5.4E-06

STOCHASTIC MEAN DOSE RATE AT SELECTED TIMES (TABLE D1 OF QUESTIONNAIRE)

	5000	10000	50000	100000	500000	1000000 a
A EMOS4	2.2E-06	3.8E-05	1.4E-05	7.4E-06	1.0E-05	8.7E-06
B JAERI-1.4	2.2E-06	4.5E-05	1.3E-05	6.1E-06	7.9E-06	5.9E-06
C LISA-1A/CI	9.6E-07	4.9E-06	1.0E-06	1.2E-06	1.8E-06	1.1E-06
D SIMPAR-2.0	8.5E-06	1.2E-05	1.3E-05	1.9E-05	2.5E-05	2.0E-05
E LISA-1A/JRC	2.8E-06	4.0E-05	1.4E-05	7.4E-06	9.8E-06	7.9E-06
F MASCOT-3	4.6E-06	5.8E-05	1.6E-05	6.8E-06	8.8E-06	8.0E-06
G STRAW-1.1	N.C.	N.C.	N.C.	N.C.	N.C.	N.C.
H SYVAC/FI	7.6E-07	6.6E-06	5.5E-07	7.3E-07	1.8E-06	1.1E-06
I VANDAL-1.2C	2.1E-06	2.6E-06	3.5E-06	3.3E-06	1.9E-06	1.3E-06
J (E)LISA-01	1.6E-06	4.0E-05	9.5E-06	4.7E-06	8.3E-06	6.8E-06
K NEFTRAN-B.2	4.0E-08	1.2E-05	4.6E-06	4.0E-06	N.C.	N.C.
L SYVAC3-L1A	1.5E-06	4.2E-05	1.8E-05	9.1E-06	2.4E-05	2.1E-05

STOCHASTIC STANDARD DEVIATION (TABLE D1 OF QUESTIONNAIRE)

	5000	10000	50000	100000	500000	1000000 a
A EMOS4	1.1E-05	9.1E-05	5.2E-05	2.6E-05	2.7E-05	2.2E-05
B JAERI-1.4	1.1E-05	1.1E-04	4.4E-05	2.1E-05	2.4E-05	1.8E-05
C LISA-1A/CI	3.8E-06	1.4E-05	2.6E-06	4.8E-06	3.6E-06	2.0E-06
D SIMPAR-2.0	1.6E-05	2.5E-05	6.4E-05	1.3E-04	1.8E-04	1.5E-04
E LISA-1A/JRC	1.5E-05	1.0E-04	5.7E-05	2.6E-05	2.2E-05	1.6E-05
F MASCOT-3	2.8E-05	1.4E-04	6.5E-05	2.3E-05	2.2E-05	1.7E-05
G STRAW-1.1	N.C.	N.C.	N.C.	N.C.	N.C.	N.C.
H SYVAC/FI	3.9E-06	1.4E-05	1.4E-06	3.4E-06	4.5E-06	2.2E-06
I VANDAL-1.2C	9.0E-06	9.7E-06	1.1E-05	9.5E-06	6.2E-06	3.9E-06
J (E)LISA-01	4.6E-06	9.6E-05	2.3E-05	9.5E-06	1.5E-05	1.3E-05
K NEFTRAN-B.2	1.5E-07	3.5E-05	1.2E-05	6.6E-06	N.C.	N.C.
L SYVAC3-L1A	6.8E-06	1.1E-04	5.8E-05	3.1E-05	7.4E-05	6.4E-05

STOCHASTIC LOWER CONFIDENCE BOUND (TABLE D1 OF QUESTIONNAIRE)

	5000	10000	50000	100000	500000	1000000 a
A EMOS4	6.4E-07	2.5E-05	6.2E-06	3.7E-06	6.2E-06	5.7E-06
B JAERI-1.4	6.5E-07	2.9E-05	6.8E-06	3.1E-06	4.5E-06	3.3E-06
C LISA-1A/CI	0.	0.	0.	0.	2.0E-07	1.6E-07
D SIMPAR-2.0	1.4E-06	6.0E-07	0.	0.	0.	0.
E LISA-1A/JRC	0.	2.0E-05	2.4E-06	2.2E-06	5.4E-06	4.7E-06
F MASCOT-3	6.0E-07	3.8E-05	7.0E-06	3.5E-06	5.7E-06	5.6E-06
G STRAW-1.1	N.C.	N.C.	N.C.	N.C.	N.C.	N.C.
H SYVAC/FI	2.1E-07	4.6E-06	3.4E-07	2.6E-07	1.2E-06	7.7E-07
I VANDAL-1.2C	1.0E-06	1.5E-06	2.2E-06	2.1E-06	1.1E-06	7.9E-07
J (E)LISA-01	0.	0.	2.0E-08	7.6E-07	2.3E-06	1.3E-06
K NEFTRAN-B.2	0.	0.	0.	0.	N.C.	N.C.
L SYVAC3-LLA	5.3E-07	2.6E-05	9.2E-06	4.6E-06	1.3E-05	1.2E-05

STOCHASTIC UPPER CONFIDENCE BOUND (TABLE D1 OF QUESTIONNAIRE)

	5000	10000	50000	100000	500000	1000000 a
A EMOS4	3.8E-06	5.1E-05	2.1E-05	1.1E-05	1.4E-05	1.2E-05
B JAERI-1.4	3.8E-06	6.1E-05	1.9E-05	9.0E-06	1.1E-05	8.5E-06
C LISA-1A/CI	2.9E-06	1.1E-05	2.2E-06	3.4E-06	3.4E-06	1.9E-06
D SIMPAR-2.0	1.6E-05	2.3E-05	4.1E-05	7.7E-05	1.1E-04	8.7E-05
E LISA-1A/JRC	5.8E-06	6.0E-05	2.5E-05	1.3E-05	1.4E-05	1.1E-05
F MASCOT-3	8.6E-06	7.8E-05	2.5E-05	1.0E-05	1.2E-05	1.0E-05
G STRAW-1.1	N.C.	N.C.	N.C.	N.C.	N.C.	N.C.
H SYVAC/FI	1.3E-06	8.6E-06	7.5E-07	1.2E-06	2.4E-06	1.4E-06
I VANDAL-1.2C	3.1E-06	3.8E-06	4.9E-06	4.4E-06	2.6E-06	1.7E-06
J (E)LISA-01	3.7E-06	8.1E-05	1.9E-05	8.6E-06	1.4E-05	1.2E-05
K NEFTRAN-B.2	1.7E-07	4.3E-05	1.5E-05	9.9E-06	N.C.	N.C.
L SYVAC3-LLA	2.5E-06	5.7E-05	2.6E-05	1.4E-05	3.4E-05	3.0E-05

NOTES

- An entry 'N.C.' indicates a result that was not calculated.
- An entry '-' indicates where the answer could not be given (eg solubility limit not reached).
- All numbers are quoted in scientific notation to 2 sig. fig.
- All dose rates smaller than 1.0E-15 Sv/a are quoted as zero.
- All times greater than the cut-off of 1.0E+6 a in table C2 of the questionnaire are entered as >1.0E+6.
- In the answers in table C3 of questionnaire, where the dose rate curve was still rising at the cut-off time of 1.0E+6 a then the time of peak is entered as 1.0E+6 a (ie the time of peak dose rate within the time-span of the problem) and the dose rate is given at that time.
- Chebychev confidence bounds are given for the stochastic results.
- These data are obtainable in machine-readable form from the NEA Data Bank, F-91191 Gif-sur-Yvette CEDEX.

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This report describes an international code intercomparison exercise conducted by the NEA Probabilistic System Assessment Code (PSAC) User Group. The PSACOIN Level 1A exercise is the third 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. Level 1A is based on a more realistic system model than that used in the two previous exercises, and involves deep geological disposal concepts with a relatively complex structure of the repository vault. The report compares results and draws conclusions with regard to the use of different modelling approaches and the possible importance to safety of various processes within and around a deep geological repository. In particular, the relative significance of model uncertainty and data variability is discussed.

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