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

PSACOIN LEVEL 2 INTERCOMPARISON

Probabilistic System Assessment Group (PSAG)

June 1994

Nuclear Energy Agency
Organisation for Economic Co-Operation and Development

Preface

The NEA Radioactive Waste Management Committee (RWMC), established in 1975, is an international committee of senior government representatives with responsibilities for scientific and regulatory policy in the field of 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 RWMC programmes 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 Group (PSAG) was established by the RWMC in January 1985 to help co-ordinate the development of probabilistic safety assessment codes in member countries. Since its establishment, the Group has met regularly to exchange information, to discuss topical issues, and to conduct code intercomparison exercises. The Group is being terminated in 1994.

A suite of probabilistic safety assessment (PSA) exercises have been carried out by the Group. These have provided participants the opportunity to compare methodologies and results, broadening their knowledge and experience, and building confidence in the use of the various codes developed for assessment studies. These exercises are referred to as Probabilistic Safety Assessment Code Intercomparisons (PSACOIN). The Level 2 exercise, described and summarised here, is the sixth in the series of code intercomparison studies undertaken by the Group and published by the OECD/NEA. The preceding five exercises are Level 0, Level E, Level 1a, Level 1b and Level S.

The conclusions presented in this report are those of the PSAG and do not express the official views of any NEA Member country or international organisation.

Acknowledgements

This document was prepared and edited on behalf of PSAG by a Task Group, as indicated on page 6 of this report.

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PSACOIN LEVEL 2 INTERCOMPARISON

Executive Summary

The Probabilistic Systems Assessment Group (PSAG) was established in 1985 by the Nuclear Energy Agency (NEA) of the Organisation for Economic Co-operation and Development (OECD). The principal purpose of the 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, discussion of topical issues, code development and code intercomparisons.

One of the PSAG's major activities has involved a series of code intercomparison exercises known as PSACOIN (PSA Code Intercomparison). The Level 2 exercise, described and summarised here, is the sixth in the series of code intercomparison studies undertaken by the Group. The preceding five exercises are Level 0, Level E, Level 1a, Level 1b and Level S.

The earlier PSACOIN exercises used relatively simple system models, and were focused on verification of the participating codes. In order to increase confidence in the use of the models, a succession of increasingly more 'realistic' exercises was envisaged:

- In the sense of representing the chemical and physical processes more accurately.
- In the sense that the models used were those likely to be used in actual national assessment calculations.
- With selection of models and data values and distributions, in such a way as to represent realistic bodies of experimental and expert-elicited information regarding a specific site.

The PSACOIN Level 2 exercise provided an opportunity to progress simultaneously along all three of these pathways. The objectives of the initial stage of the exercise were:

- To assemble model treatments of a single system using a variety of conceptual models for radionuclide transport, and thus to explore the effect of conceptual model uncertainty.

- To study for different performance measures the relative impact of conceptual model uncertainty.

- To study methods for the derivation of probability density functions (PDFs) for model parameters, and to explore how this process interacts with the range of conceptual models considered.

Later stages were to study progressively the effect of incorporating conceptual model uncertainty into different components of the system, e.g., groundwater flow in Stage 2 of the exercise.

The scope of the Stage 1 exercise was deliberately limited:

- It was only possible to illustrate the range of variability in results from the alternative conceptual models used by the participants. It was not possible to assess the uncertainty from the lack of completeness of the set of alternative conceptual models.

- Participants were provided with interpreted data - such as values of K_d (as opposed to 'raw' data). A particular conceptual model already stands behind any interpreted data. Provision of interpreted data may have limited the ability to consider as broad a range of alternative conceptual models as might be considered in a real assessment exercise.

- More complex modelling approaches require greater resources than simpler modelling approaches. Resource limitations may have limited the range of models considered, compared to the range that would be considered in a real assessment exercise.

Conclusions

Given the scope of the exercise, how much was achieved? A set of conclusions is presented here that address the original objectives of the Level 2 exercise.

Alternative conceptual models used

Alternative model treatments were assembled for radionuclide transport; these ranged from fracture-only transport models, to equivalent porous media models, to dual-porosity models, to matrix-only transport models. Both one-dimensional and two-dimensional approximations were used. None of the models were judged to be inconsistent with the limited information on radionuclide transport in the Culebra Dolomite provided in the Problem Specification. Of course, in a real assessment exercise, it may be possible to assemble information that could limit the range of conceptual models to a much greater degree than could the information provided in the Level 2 Problem Specification.

The range of models used was based on the in-house capabilities and codes of the participating organisations, and national regulatory backgrounds.

Importance of 'accessible' porosity

Results submitted by the different participants varied widely. The wide range of results for given performance measures was attributable to the different conceptual models used by the participants, the different numerical approximations made, and the different treatment of parameter uncertainties, in order of decreasing importance. Many of the differences can be qualitatively explained. The largest single determinant of results was the assumption made concerning the 'accessible' porosity. Transport models accounting only for fracture porosity led to much more rapid and greater releases and doses than transport models that accounted for physical retardation through rock matrix diffusion. Given the information in the Problem Specification, rock matrix porosity dominated in the equivalent-porous media, dual-porosity, and matrix-only models.

Importance of numerical approximations

A large range of numerical approximations and approaches were used by the participants. The potential impact of these approximations on the results needs to be understood before the issue of conceptual model uncertainty can be addressed. The main approximations of concern were:

- Approximations made in defining the boundaries at which the performance measures were calculated.
- Approximations made in gridding.
- Approximations to temporal discretisation.
- Sample size.
- Dimensionality.
- Approximations to the flow field.

- Unintended parameter correlations.
- Numerical algorithms.

Importance of conceptual model uncertainty

The definitions developed by the PSAG for the terms 'conceptual model', 'alternative conceptual model', and 'conceptual model uncertainty' seemed broadly workable. A model is defined as a set of assumptions consistent with available information within the context of a given purpose. For the purpose of the PSACOIN Level 2 exercise, the difficult aspects of this definition were defining the 'purpose' of the analysis and assessing 'consistency':

unfortunate phrasing

- The exercise did not have a 'purpose' in the sense of providing a yardstick against which the significance of conceptual model uncertainty could be compared. In a real assessment exercise, yardsticks would be available in the form of national regulatory criteria. Lacking a yardstick of this kind, any international exercise based on a hypothetical disposal case will be unable to come to terms with the significance of uncertainties, be they primarily related to conceptual models or individual parameters. For example, it may not matter if alternative models give results that differ greatly if the most conservative set of results is below the specified performance criteria - provided that the differences between model results can be explained.
- All of the models used by participants were considered to be credible, in the sense that they could not strictly be shown to be inconsistent with the available information. But consistency can only be assessed once the purpose of the modelling activity is clearly specified. Does it make sense to talk about conceptual model 'uncertainty' when comparing the results of a conservative model with those of a model aiming at a representation of the system that accounts for the actual physics in a more realistic way?

processes

Thus, given the limited constraints on modelling of radionuclide transport in the Problem Specification, the results of the Level 2 exercise demonstrated that a variety of conceptual models could be defended, and that their use leads to large differences in results. Furthermore, the range of models used gave results that are likely to bound the particular problem studied. For example, cumulative releases at the 5 km boundary ranged from release of the entire inventory at close to the speed of groundwater transport (i.e., limited retardation), to no releases in the 10,000-year time frame studied, depending primarily on the model assumptions concerning accessible matrix porosity. Additional data - in particular concerning accessible porosity - would be required to constrain the range of conceptual models used.

Relationship between parameter uncertainty and model uncertainty

It was originally intended to study the relationship between these two types of uncertainty within the Level 2 exercise. However, in Stage 1, all but one of the participants used the PDFs provided in the Problem Specification. Issues concerned with the process of constructing PDFs were not explored, and this objective of the exercise was not fully met in Stage 1.

Recommendations

Several conclusions can be drawn and corresponding recommendations made based on the results and conduct of the Level 2 exercise. However, given that this exercise will be the last in the series of PSACOIN exercises that has extended over the past decade, an effort has been made to integrate the experience gained from conducting the entire suite of exercises in developing this set of recommendations.

Resource requirements

Sufficient resources need to be made available to ensure that unambiguous results are achieved. The earlier PSACOIN exercises could be done well by individual modellers working relatively independently. However, a decade on from the initiation of the PSAG, most of the meaningful tasks that could be accomplished easily at international level have been completed. The level of complexity of the exercises has correspondingly risen so as to require teams of participants, with a variety of expertise. In general, for a fruitful exercise, each team would need expertise in several of the areas required for a national assessment. These areas might include the geosciences, numerical modelling, and system assessment.

Any new international exercises should explicitly call for the integration of a wider range of expertise, if they are to carry the potential of substantial benefit. The resource requirements will be higher within each participating organisation than in previous exercises, where individual modellers could contribute successfully. The complexity of the information resulting from such exercises will also require greater resources for the technical co-ordination, analysis and reporting of the work.

Priorities

A related lesson concerns the level of priority provided international modelling exercises. Such exercises cannot be expected to succeed if they are not accorded sufficient priority within the participating organisations. In our view, international exercises provide unparalleled opportunities for technical peer review of national modelling activities. The most important benefits of the PSACOIN exercises - Level 2 included - have been the opportunities provided for participants to find errors in their codes, to confront their own biases on a variety of aspects of system assessment modelling, and to broaden their thinking on the key aspects of system assessment modelling.

Conceptual model uncertainty

The PSAG has spent several years grappling with the issue of conceptual model uncertainty, both at a philosophical level and at the level of trying to design and conduct a concrete exercise to understand the potential importance of these uncertainties in a system assessment. Other international groups have also considered the issue of conceptual model uncertainty, and further work at international level is strongly recommended. In particular, a framework for consideration of conceptual model uncertainty is still required. For example, in the PSACOIN Level 2 exercise, a variety of modelling approaches was used. One participant aimed intentionally at a conservative treatment of the uncertainties in the available data, and used a model of fracture-only transport, leading to extremely rapid releases. This approach was considered to be acceptable within the purpose of the exercise, because information was not available that would rule out this class of model. Yet when conservative models are considered, it becomes difficult to distinguish between a model uncertainty, and an assumption made for the purpose of demonstrating compliance with a regulation.

Iteration

All international modelling exercises require more than one round of analysis and evaluation of results, if they are to achieve a successful completion. In planning the PSACOIN Level 2 exercise, two (or more) iterations were foreseen. However, the disbanding of the PSAG prevented a continuation of the exercise at an international level. In the event, the first iteration of the Level 2, Stage 1 exercise illustrated an important feature of all such exercises: inconsistencies in results led to the identification of errors in the submissions of several participants.

Of course, there is also a lesson of wider interest here. All PSACOIN exercises have required several iterations of evaluation of results and recalculation. All future modelling intercomparisons will require this kind of iteration. National assessments can be seen in the same light. Performance assessments should be conducted iteratively within a site evaluation project, and they should receive external review, to help identify potential errors and uncertainties in the assessment results. Independent assessment teams have been established by several national regulatory organisations to provide a further check on the validity of assessment results. This represents a kind of national assessment comparison exercise.

Model complexity

The range of transport models used in the Level 2 exercise included both one-dimensional and two-dimensional approaches. The one-dimensional approaches had the advantage that many simulations could be made quickly, and the participants could respond rapidly to requests for further information or additional calculations. The two-dimensional approaches had the advantage that they accounted for the actual physics of the problem in a more realistic manner, thus providing a better picture of the sensitivity of system performance to various features of the system. However, it was more resource intensive and time consuming for the participants with two-dimensional models to provide additional calculations.

A compromise approach was proposed by the Task Group, but there was no opportunity to test its validity. This approach would entail the use of a one-dimensional model to perform the bulk of the probabilistic analyses, combined with a two-dimensional model that would be run deterministically with values for the uncertain parameters selected based on the results of the one-dimensional analyses. The main role of the two-dimensional analyses would be to confirm the validity of the simpler one-dimensional analyses. This type of approach was used successfully in an inverted sense by one participant (AEA/I): two-dimensional analyses were conducted in advance of the one-dimensional analyses, with the purpose of calibrating the one-dimensional analyses.

Performance measures

The complexity of the exercise required the provision of information in electronic form to participants, and the calculation of many performance measures. Thirty-five different cumulative distribution functions (CDFs) were requested of participants, in addition to deterministic results and sensitivity analyses. It was difficult to know *a priori* which of this information would prove of benefit in understanding the outcome of the exercise. In the event, not all of the requested information was used in the intercomparison. For example, peak releases and doses could not be used because, for many simulations, the peaks occurred after the 10,000-year cut-off used by most participants. The use of electronic means of data transfer facilitated the provision and interpretation of the large amounts of information requested, and the Task Group found this of value.

Additional information was identified that might have been of further value in understanding the results of the exercise, but that was not requested in the Problem Specification. For example, plots of breakthrough curves and release against time should be considered in future such exercises. A full CDF of the time of peak release would have shown broad trends without risking distortion of mean values by the cut-off of values greater than the limit set by the time to which simulation proceeded.

ATTACHMENT 5

SAMO '95

Symposium on Theory and Applications of Sensitivity Analysis of Model Output (SAMO) in Computer Simulation

Belgirate (I), 25-27 Sept. 1995.

From: SMTP%"andrea.saltelli@cen.jrc.it" 14-JUN-1994 17:07:07.61
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Subj: SAMO '95 advertising at next PSAG meeting, 16th June, Paris

Posted-Date: Tue, 14 Jun 1994 17:02:39 +0200 (DFT)
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Foreword

Dear Member of PSAG

I am presently working on a project for a symposium on Sensitivity Analysis of model output, which shall be held at Belgirate, on Lake Maggiore (I) on September 1995. At present the project is advanced enough for me to dare to submit it to you, although many things in it are still provisional. Apparently the project will be jointly financed by the Joint Research Centre and by the European Commission, Directorate General XII (Science, Research and Development) of Brussels. Unfortunately I cannot attend this PSAG meeting to promote the symposium. On the other hand I am confident that Enrico Sartori, to whom I am indebted for the acronym of the conference, will be a very effective salesman.

To my recollection the members of the PSAC, then PSAG group have animatedly argued on sensitivity analysis issues twice a year for a period of ten years, clearly showing that there is no international consent on sensitivity analysis methods and strategies. My main concern, in submitting this project to you, is to have all the voices raised within PSAG represented at this conference. I am well aware of the incompleteness of the present document. There are probably important omissions, which you can help me to remedy. A few investigators, listed in the scientific organising committee, have already given their assent to the project, but the list is an open one. I welcome your proposals. Similarly, the list of invited papers reflects my present patchy knowledge of the literature, which you can invigorate with fresh suggestions.

Provided that the financial details are sorted out, I expect to send out a first announcement before the end of this summer. All of you will be kept timely informed.

I hope you find this project stimulating for your discussion at the PSAG meeting. I also hope to see you at the symposium next year.

A. Saltelli

SAMO '95

Symposium on Theory and Applications of Sensitivity Analysis of Model Output (SAMO) in Computer Simulation

Belgirate (I), 25-27 Sept. 1995.

Organisation and objectives. The symposium is promoted by the Environment Institute of the Joint Research Centre of the European Commission (EC), together with the Directorate General XII Science, Research and Development of the EC. The purpose of the initiative is to bring together people from different disciplines involved in practical and theoretical aspects of Sensitivity Analysis (SA). Another objective of the symposium is to give a wider audience to interesting recent developments in the field of SA.

A working definition. The objective of sensitivity analysis of model output could be defined as the quantification of the relative importance of each input model parameter in determining the value of an assigned output variable. More specifically global SA aims to apportioning the uncertainty in the output prediction to the uncertainty in each input parameter. Sensitivity analysis fades into uncertainty analysis. It is not always possible to separate the two.

The applications. Although sensitivity analysis applies to all branches of modelling and computer experiments, it does not seem to be a fully established discipline of its own yet, possibly because it is very much application driven. New techniques are developed by researchers in different branches, from chemical kinetics to reactor and nuclear waste safety, from environmental impact assessments to global change studies. SA can also be crucial in economics, with existing applications to financial and economic evaluation of investment plans. SAMO can be effectively used for model validation and QA, model calibration in presence of uncertainties and model performance comparison. The model added value which SAMO can produce is very high.

In the past a series of international exercises of model comparison (including SAMO) have been undertaken by an international organisation, the Organisation for the Economic Cooperation and Development (OECD), in the field of nuclear waste disposal (Nuclear Energy Agency of the OECD, 1987, 1993). One of these exercises, named Level S, and promoted by the Probabilistic System Assessment Group (PSAG) of OECD-NEA was focused on comparing the performances of different SA techniques on a selected test case.

The EC also pioneered the use of SA in Europe with its PAGIS, PACOMA and EVEREST projects (PAGIS, 1989).

Cross fertilisation. Given the potential impact of SA on model performance, its use should be encouraged and its results brought to the largest audience. The workshop wishes to be a step in this direction, aiming to bring together various scientific communities active on SA from different disciplines and countries.

Anything new? Many interesting developments in SA have been made in recent years. A short non-exhaustive list of new developments, which the symposium should disseminate, would include:

- A recent original work in the field of global sensitivity analysis of Welch et al., (1992) on efficient parameter screening, based on data adaptive modelling;
- Progresses made by Andres and Hajas, (1993) using Iterated Fractional Factorial Design, for system with many (thousands) uncertain parameters. Also interesting in this field is the work of Bettonvil and Kleijnen (1991).
- Advances on a new measure of importance for SA develped by Hora and Iman (1986, 1990); Ishigami and Homma, (1989, 1990); Saltelli et al., (1993).
- The introduction of the sensitivity indices, (Sobol' 1990), which can be viewd as a generalization of the importance measure and have analogies with the FAST method.
- An approach to SA due to Cawlfield and Wu (1993), where probabilistic SA is performed within the frame of First Order Reliability Analysis (FORM).
- A sensitivity analysis method for stochastic differential equations developed by M. Koda (1992).
- Possibly the most fertile school of sensitivity analysis is that active at the SANDIA National Laboratory in New Mexico. A recent review of SA methods, covering also plenty of SANDIA work, is that of Helton, (1993).

A possible outline of the conference sessions.

1. Identifying active factors in large batches
2. Importance measures and Fourier Amplitude Sensitivity Tests
3. Correlation / regression based techniques and surface replacement
4. Local sensitivity analysis
5. Applications

Scientific Organizing Committee (so far). Prof. J. C. Helton, Department of Mathematics, Arizona State University, Tempe, AZ, USA. Prof. I. M. Sobol', National Center for Mathematical Modelling of the Russian Academy of Science, Moscow, CIS. Prof. J.P.C. Kleijnen of the Tilburg University, NL. Dr. E. Hofer, Gesellshaft fur Anlagen und Reaktorsicherheit (GRS), Garching, D. Dr. M. Scott, Department of Statistics, University of Glasgow, UK. One project leader to be designated from DG XII, Brussels. Dr. A. Saltelli, Environment Institute, Joint Research Centre of Ispra, (I). An invitation has been sent to Prof. S. C. Hora, Division of Business Administration and Economics, University of Hawaii at Hilo, USA.

Ideas for invited papers (so far). T. H. Andres on Iterated Fractional Factorial Design (IFFD). J.P.C. Kleijnen and B. Bettonvil on parameter identification. One or more selected speakers among Welch, W. J., Buck, R. J., Sacks, J., Wynn, H. P., Mitchell T. J., and Morris M. D. on their recent developments. R. L. Iman and/or S. C. Hora on importance measure. E. Hofer for an application of this measure. One or more speakers to be selected among Dunker, A., Dougherty, E. P., Hwang, J.T., and Rabitz, H. for local SA. I. M. Sobol' on sensitivity indices. T. Homma on the same subject. R. L. Iman and/or J. C. Helton on correlation /regression based sensitivity analysis techniques. One or more speaker to be selected among Cukier, R. I., Levine H. B., Schuler C. M, Liepman, D. and Stephanopoulos, G., Mc Rae, G. J. on FAST. One speaker to be selected among Cawlfield J. D. and Wu, M.C. on First Order Reliability Method (FORM) in sensitivity analysis. One speaker to be selected among Vajda S., Valko, P., and Turanyi T. on principal component analysis in local sensitivity analysis. One speaker to be selected among Alcamo, J., and Bartnicki, J. on the use of SAMO on models of environmental impact. One or more selected speakers among E. Hofer, J. Marivoet, J.P.C. Kleijnen on EVEREST (an international exercise on SA). One or more speaker to be selected among A. Alonso, P. Robinson, E. J. Bonano, and D. A. Galson about the OECD Level S exercise (ditto).

Other data on the symposium. The conference's target is between 40 and 50 papers. Posters will be also considered. The expected number of participants is of the order of one hundred. In general oral presentations (with no written support) will be discouraged. The proceedings will be published (from Kluwer, Dordrecht, NL). A selected subset of the contributions will form a Special issue in the Journal of Statistical Computation and Simulation. Dr. M. Scott, associated editor of this Journal, has already contacted to this effect the editor who has welcome the proposal. Participation fee will be in the range 170 - 230 ECU (200 - 270 US$) and will cover lunches, coffees and transportation. Hotel expenses will be covered by participants.

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ATTACHMENT 6