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Research

# Radionuclide Transport Modelling: Current Status and Future Needs

Seminar Johannesberg, Sweden, 6-8 November 2001

**Synthesis, Work Group Reports and Extended Abstracts**

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## Foreword

As part of preparations for review of future license applications, the Swedish Nuclear Power Inspectorate (SKI) and Swedish Radiation Protection Institute (SSI) convened a joint workshop on radionuclide transport modelling, held 6-8 November 2001. The principal objectives of this workshop were to identify the present status of SKI/SSI capabilities relating to radionuclide transport modelling, and to generate a list of actions to prepare for reviews of future performance assessments in conjunction with radioactive-waste repository license applications. These discussions will provide a basis for planning of future research and development activities. It should be noted that this planning is only related to the activities that the authorities will perform independently and that the content of this report is not directly related to the activities of the implementor. This report includes a synthesis of the main workshop findings as well as reports from several working groups addressing key topics related to radionuclide transport. In order to address practical details related to this, some views had to be expressed that related to the superordinate topic of developing a strategy for reviewing future performance assessments.

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# 1. Introduction

The Swedish high-level radioactive waste repository programme is moving into a new phase, with the start of site investigations by the Swedish Nuclear Fuel and Waste Management Co. (SKB) in the spring of 2002. Based on these investigations, a license application for permission to proceed with subsurface investigations at a potential high-level repository site could be submitted as soon as 2007, according to SKB's timetable (SKB, 2001b). These present and future steps necessitate preparations for developing the review capability of the Swedish regulators (SKI and SSI). The main purpose of the workshop was to identify the present status of SKI/SSI capabilities relating to radionuclide transport modelling and suggest how this capability can be updated and developed.

The workshop took a broad perspective on the issue of radionuclide transport modelling including related topics such as the source term, i.e. release of radionuclides, groundwater flow in the geosphere, and biosphere exposure pathways. The seminar did not aim to address issues pertaining to degradation of engineered barriers, which will be the focus of other SKI activities. Site-characterisation issues were not a central focus of the radionuclide transport modelling workshop, but were discussed in a separate seminar (SKI, 2001), which included many experts who participated in the workshop.

This report presents the findings of this workshop, and a first synthesis of the findings in terms of recommended directions for work in preparation for reviews of future performance assessments. This synthesis emphasises issues related to radionuclide transport, but is intended to contribute to the more general framework for preparing for future review efforts. In writing this synthesis, comments from various sources within SKI/SSI have been considered, in addition to suggestions made by the workshop participants. However, the main sources of information are the appended reports of the working groups (Appendix 2-7), and the appended abstracts by individual experts who gave presentations (Appendix 9).

This report mainly discusses future and present preparations for future performance assessment submissions and eventually the licensing processes. The planning for the actual licensing and review phases is beyond the scope of this report, but is referred to in places to illuminate the context for other issues.

# 2. Background

The efforts of SKI and SSI to prepare for an eventual review of a license application for a deep repository and an encapsulation plant have been ongoing for two decades, and thus it should be emphasised that these efforts are not just beginning now. However, the research-oriented perspective that prevailed in the early stages has shifted gradually toward issues more directly related to review methodology as well as their ultimate implementation, and eventually compliance evaluation.

SKI's and SSI's programmes should give access to necessary expertise to assist SKI/SSI in its review work. The experts affiliated to the authorities must be able to address all detailed scientific technical issues that are of relevance for long-term as well as operational safety.

SKI has previously allocated significant resources for developing independent performance assessments, which included development of capabilities for independent modelling. The outcome of these efforts has been documented in two performance assessment reports (Project-90 and SITE-94). As the Swedish programme is now approaching an implementation phase, it is not possible to prioritise major development projects and it is consequently necessary to place a larger emphasis on using and updating what the authorities have previously developed. These efforts need to be focused on specific goals, such as implementation of regulations and guidelines, SKB's site characterisation work and SKB's performance assessment projects. It will be necessary to gradually focus more and more attention on finding the sufficient level of knowledge about all relevant topics. The review of SR97 by SKI and SSI (SKI, 2000a), supported by in-depth expert reviews (SKI, 2000b), provides a good starting point for assessing SKB's viewpoints and priorities in the area of performance assessment. This will form a basis for development and updating of the review capability of the authorities.

An important issue during the extended research, development and implementation period for the planned Swedish spent fuel repository, covering several decades, will be to maintain, develop and extend the competence level of the experts engaged by the authorities. These experts need, in addition to their knowledge in technical and scientific areas, to have a good knowledge of the specific regulatory context in order to provide input of direct relevance for regulatory work. They also need to be up to date regarding ongoing activities in the Swedish programme, which will be important for their motivation and interest in SKI/SSI work. Since the specific importance of various technical areas will vary through the different stages of the SKB programme, SKI and SSI need to be continuously aware of possible needs, to cover new areas and to engage additional experts. However, the experiences so far indicate that best results and the most relevant regulatory viewpoints have often been obtained in cases where the collaboration with external experts has occurred over at least a few years. Basic agreements could be made between SKI or SSI and various organisations providing support. However, an informal long-term collaboration with external experts has been and will probably continue to be the most widely used option.

## 3. Workshop Objectives

The main objectives of this workshop were to gain an overview of the state-of-the-art in radionuclide transport modelling with special attention to review contexts, and to generate a list of actions and needs for SKI and SSI to prepare for a performance assessment submission. Basic questions addressed by this workshop included:

- What is practical to do today?
- What critical needs exist?
- What ideas should be carried through over a 3 to 5 year perspective?

The workshop discussions were aimed at identifying key issues, including issues where more focused workshops might be needed, with an objective to produce "position papers" on these specific topics.

## 4. Workshop Organisation

To facilitate discussion of the broad range of topics that pertain to radionuclide transport, the workshop participants were organised into working groups to discuss specialised topics. In the first two days of the workshop, working groups focused on three main divisions of the repository system:

- Near field
- Far field
- Biosphere and risk evaluation

Each working group was asked to respond to a series of questions which were provided as a guide to discussion, but the working groups were also encouraged to identify key issues that were not raised as questions. Summaries of the main findings of these working groups were presented in a plenary session.

On the third day of the workshop, three different working groups were formed specifically to address integration issues and interactions between the divisions previously considered:

- Integration and overall strategy
- Near-field/far-field interactions
- Far-field/biosphere interactions

The findings of these working groups were presented in a plenary session. Following this, the workshop concluded with a discussion of the key issues that the workshop participants agreed should receive high priority in preparations for future reviews of performance assessments (listed in appendix 1). Summaries of the discussions within the working groups and plenary sessions are presented as appendices to this report (appendix 2-7).

## 5. Synthesis of Workshop Results

A key need identified in the workshop was the need for a comprehensive review strategy, so that the authorities can formulate concrete plans for effective utilisation of their limited resources, in carrying out an effective review. In this context, the results of the workshop can be addressed in terms of the following broad topics:

- Structure for organising expert participation
- Performance assessment strategy and review context
- Priorities and ambition level for reviews
- Analysis of repository system and scenarios
- Role of SKI/SSI models in performance assessment reviews
- Role of SKB models in SKI/SSI reviews
- Needs for development of specific modelling capabilities

These topics are discussed in turn in the following sections.

### 5.1 Structure for organising expert participation

The working group on *review integration strategy* (appendix 5) proposed the use of *clearinghouses* or expert groups as a mechanism for effective utilisation of the available expertise. The clearinghouses would not act independently but would work in close collaboration with the authorities. SKI and SSI personnel could in some cases also be included in these groups. Their main tasks would be to follow the Swedish programme, to single out critical topics for review or project work, as well as to provide general advice to the authorities about relevant technical aspects of deep disposal. The groups would have meetings on a regular basis, so those experts would have an opportunity to communicate with each other, and to develop up-to-date opinions on the overall status of the Swedish programme.

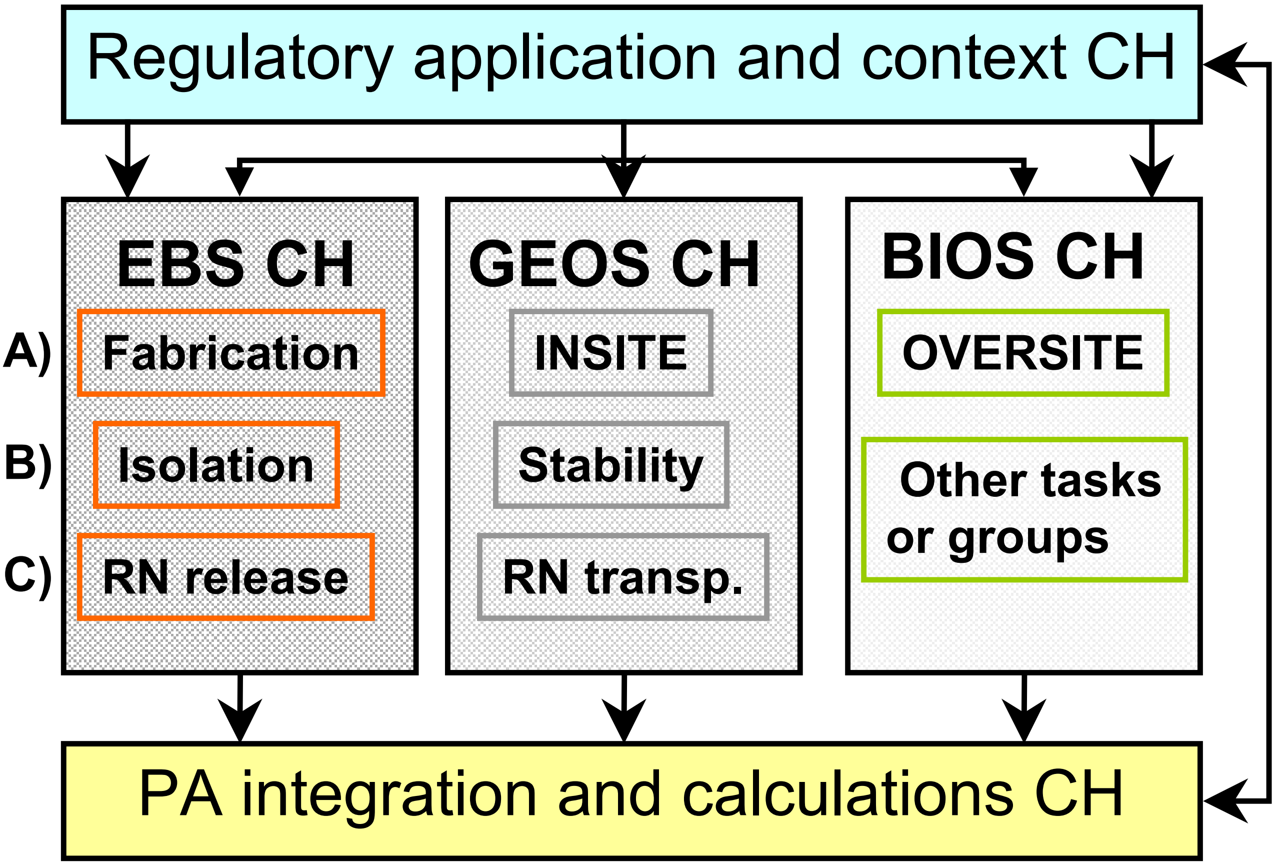


***Figure 1*** Proposed clearing houses for future review efforts. The top clearing house will address issues related to regulatory policy. The bottom clearing house will address integration and the authorities independent modelling capability. The three central clearing houses will address the three main scientific and technical areas, engineered barrier system, geosphere and biosphere; EBS CH = Engineered Barrier System Clearinghouse. GEOS CH = Geosphere Clearing house. BIOS CH = Biosphere clearing house. The subgroups at the top of each central box correspond to the site and repository specific part (denoted A). The subgroups in the middle address the system understanding part as a basis for performance assessment (denoted B; e.g. isolation of radionuclides by engineered barriers and stability of geosphere). The lowest subgroups address the fate of escaping radionuclides and is directed to quantitative analysis of consequences (denoted C). The INSITE and OVERSITE groups are already established for reviewing SKB´s site characterisation efforts. Other groups and tasks are preliminary.

Upon further consideration, we here propose a list of five clearinghouses (Figure 1), which are slightly modified from the six clearinghouses proposed by the *review integration strategy* group. The external experts should complement each other in terms of technical expertise and should be independent from SKB.

The clearinghouse on *regulatory application and context* should be composed mainly of SKI and SSI personnel, and will need to address all issues pertaining to regulatory policy. The *performance assessment integration and calculations* clearinghouse should be used for maintenance and application of SKI's and SSI's own modelling capability. These two clearinghouses should communicate with each other, since the perspectives of regulatory context and overall relevance in performance assessment must be iterated. The other clearinghouses approximately correspond to the three main working groups at the seminar (near-field, far-field, and biosphere). The interfaces among these groups were briefly addressed at the workshop (see Appendix 6-7). The experts within the three main technical expert groups should be given overall direction by the *regulatory application and context* clearinghouse and should provide direction to the *performance assessment integration and calculations* clearinghouse.

The three main clearinghouses (EBS, Geosphere and Biosphere) could at suitable occasions during the next few years prepare (and possibly update) a status report covering the major performance assessment issues within the mandate of each group. The clearinghouses should consider previous reviews of SKB's RD&D programmes and other viewpoints expressed by the authorities. The status reports could be part of the ”issue resolution tool” proposed at this workshop. The main purpose of these reports would be to focus future review activities.

The authorities may need some assistance in prioritising activities within their own research and development programmes. The clearinghouses could have a limited role also in this context and could suggest a priority list, for consideration of the SKI/SSI staff, on topics that could be addressed within the SKI/SSI programme (modelling studies, reviews of a particular topic etc.).

The INSITE group (**In**dependent **S**ite **I**nvestigation **T**racking and **E**valuation) is an expert group that has already been established for following the SKB site characterisation programme. The clearinghouses for following the SKB performance assessment work should be integrated with this already existing expert group. The topics dealt with in the INSITE group will to a large extent coincide with those of the geosphere clearinghouse. The geosphere clearinghouse could be an extension of the already existing INSITE group, which would ensure feedback between aspects of site characterisation and performance assessment.

## 5.2 Performance assessment strategy and review context

Regulations recently developed by SSI are based on the concept of ***risk***, versus the concept of maximum dose, which was the previous basis for regulatory planning. There is a recognised need for the authorities to provide regulatory guidance to SKB on how to interpret the risk-based regulations in terms of performance measures.

As discussed in appendix 4 work is needed to develop guidelines for the form and presentation of risk measures, how risk is integrated in time and space, and the use of surrogate measures for risk such as concentrations in environmental media. An additional aspect to consider under the current regulations will be impacts on non-human biota. Finally, the guidelines need to address not only estimates of net risk based on the integrated repository system, but also demonstration of compliance with the multi-barrier principle.

Workshop participants concluded that the adoption of risk-based regulations implies a need for the safety case to emphasise probabilistic methods in addition to deterministic methods for consequence evaluation. However, this does not necessarily mean that a fully probabilistic approach will be the best strategy for review. A review strategy will need to address both the underlying process models and the probabilistic methodology that is used to integrate their results to yield estimates of risk. In addition, the influence of and basis for utilised parameter probability distributions requires consideration.

Issues to consider in review of a probabilistic risk assessment methodology include:

- Determination of probability distribution functions for parameters,
- Formal use of expert judgement and generic vs. site-specific data,
- Selection of scenarios and treatment of scenario probability,
- Selection and probabilistic treatment of exposed groups,
- Convergence criteria, and
- Traceability, reproducibility, and transparency of results.

Targeted, deterministic "what-if" calculations using detailed process models are still expected to be needed in the review context, to address questions about the significance of simplifications in the underlying process models, and to check compliance with the multiple-barrier principle.

## 5.3 Priorities and ambition level for reviews

An essential part of the preparations for future performance assessment reviews will be to judge the required level of effort in reviewing various parts of an SKB performance assessment and the background documentation. Since resources available to the authorities are limited, the review itself needs to be focused on critical issues, with a sufficiently detailed knowledge of background documentation as a starting point.

Status reports that are prepared and updated by the clearing houses during the preparation phases should give recommendations about points that will need to be addressed with particular attention during a review. In addition, the treatment of the issues raised in reviews of the SKB RD&D-programmes should naturally also be considered. The authorities' own modelling projects should be organised such that topics of controversial nature in SKB's background documentation are addressed. The outcome of independent modelling projects also needs to be compared with the SKB safety reporting and any significant discrepancies would naturally have to be understood and if possible resolved.

The effort required in obtaining a sufficient basis to form a regulatory standpoint about a particular safety assessment issue could vary considerably depending on e.g. the level of complexity, the level of scientific controversy, the influence on various performance measures as well as criteria for radiation protection and long-term safety. The working groups were asked to categorise different review tasks as:

- non-controversial,
- requiring expert judgement (detailed expert review)
- requiring scoping calculations (detailed expert review supported by limited scoping calculations to check SKB results) and
- requiring independent modelling (detailed expert review supported by application of SKI's independent modelling capability).

An additional, important basis for ranking the tasks will be to analyse SKB's safety-allocation principles and SKB's safety case. Topics of unresolved significance should if possible be identified early on in a review phase. Otherwise, the possibilities to analyse these with SKI's and SSI's own modelling tools would be limited. Although the review phase would have to be extended if unresolved issues unexpectedly appear, it would not be practical to extend the review phase indefinitely.

Access to independent modelling capability will require significant preparatory work in the coming years. Although SKB's performance assessments should give a comprehensive overview of all aspects related to long term safety, access to independent models would be necessary to gain additional understanding and coverage. It would be unreasonable to expect that SKB's performance assessments would by themselves give a sufficient basis for clarifying all significant aspects of long-term safety from all perspectives that a reviewer may consider. In addition, expert judgement alone cannot be expected to provide a sufficient basis for establishing a regulatory standpoint on all issues.

If particular difficulties are encountered in establishing a regulatory viewpoint about a particular topic or issue, one of the previously suggested clearing houses (see 5.1) could be used to e.g. thoroughly review the scientific background and open literature as a basis for an expert judgement covering the sufficiency of SKB's treatment in performance assessment and background documentation. These groups may in such cases have to be extended with additional members that represent scientific disciplines not represented by the presently affiliated experts. These new members could be associated on an ad-hoc basis.

## 5.4 Analysis of repository system and scenarios

System analysis is an essential tool in performance-assessment work, to demonstrate completeness of the system description and to judge the sufficiency of the representation of ***features, events, and processes*** (***FEPs***) in the mathematical models that support a particular performance assessment. The ***process influence diagram (PID)*** illustrates how the various FEPs affect each other. The ***assessment-model flow chart*** (***AMF***) is a graphical illustration of the information exchange within the various models within a performance assessment.

The essential components of a system analysis include:

- a compilation of all relevant FEPs,
- a description of the essential features of each FEP (i.e. a FEPs encyclopaedia), and
- a graphical representation of how the various FEPs are connected with each other (e.g. a process-influence diagram, PID)
- an analysis of the importance level of various FEPs and justified decisions why certain FEPs can be eliminated while others have to be accounted for.

An essential effort will be required to organise the available expertise such that the adequacy of all parts of SKB's system analysis will be covered. As a basis for SR 97, SKB summarised their system-analysis in a special process report (SKB, 1999) and developed the THMC-method for illustrating the influence between all significant processes and variables. This work will be modified and updated with every new major performance assessment.

The *Review Integration Strategy* group recommended that the systems-analysis approach should also be viewed as a regulatory tool in addition to serving as a basis for developing a performance assessment. In future review work, emphasis should be directed toward checking the sufficiency of SKB's processes and also ensuring that the treatment within the modelling part of a performance assessment is consistent with the descriptions within the process report.

In addition to this, the PID-AMF approach may be implemented in a simplistic way as a means to organise a review. As a preparation for this, SKI was recommended to finalise its own FEPs encyclopaedia and to develop further and implement the SPARTA code, in order to visualise the PID in a reasonably transparent way.

Systematic analysis of FEPs should also form the basis for selection of scenarios that should be considered in the performance assessment and review. Key issues to consider are the comprehensiveness of the set of scenarios that have been selected for evaluation, and whether potentially significant couplings between scenarios have been accounted for. In the evaluation of an integrated risk assessment, the authorities need to address the sufficiency of the justification for the assigned scenario probabilities.

## 5.5 Role of SKI/SSI models in performance assessment reviews

The development of SKI's and SSI's modelling capability need to be an essential part in preparing for future reviews of performance assessment submissions. Independent modelling capability is needed as a support for expert reviews and for raising the competence level both for SKI and SSI staff and for affiliated experts. It is also a prerequisite for demonstrating regulatory competence and to develop and clarify standards and criteria in regulations and guidelines.

The authorities have over the years utilised (and in several cases developed) performance assessment codes covering all geoscientific disciplines and parts of the combined EBS, geosphere and biosphere system. Some of these codes are tailored to particular regulatory needs, while others are general codes utilised by most organisations involved in the field.

An important conclusion from the working groups was that a review of SKI's and SSI's current modelling capability should be initiated. All codes available that might be useful in connection with future review efforts should be checked in the near future. Documentation of codes (fixed versions, user manuals etc.) and quality assurance should be improved. The most stringent requirements on quality assurance would be required if independent modelling were used to develop the framework for standards and criteria.

SKI and SSI should also develop a plan for any code development that may be needed. In order to test the usefulness of a particular code, limited performance assessment exercises could be conducted, which would ensure that the codes are well adapted and functional as well as providing a comparison with the corresponding treatment in other relevant performance assessments. SKI and SSI need to integrate their modelling tools to make sure that they are compatible and can be combined in such a way that the whole system is covered.

The calculations conducted with independent modelling tools should be set up such that any corresponding SKB analysis is considered. For instance a modelling tool might be used to quantitatively confirm any key modelling result from SKB´s safety reporting, to analyse a simplifying assumption of particular significance, to analyse parameter sensitivity or to verify safety allocation priorities. The ranking of the relative importance of various parameters could provide a very useful basis for selecting areas of laboratory work or site characterisation for detailed review. A probabilistic analysis could be used examine parameter uncertainty and various sensitivities, while conceptual and scenario uncertainty could be addressed with deterministic ”what-if” scooping calculations.

### 5.6 Role of SKB models in performance assessment reviews

In order to obtain a sufficiently detailed view of SKB’s performance assessment modelling capability, SKI and SSI need to devote more effort to scrutinising the SKB modelling tools. It is essential for the authorities to develop a general understanding of the significance of various types of uncertainties (conceptual uncertainty, parameter uncertainty, numerical uncertainty, and uncertainty stemming from spatial variability and time dependence) in the performance assessment. This is likely to be difficult without full understanding of the quantitative framework that is being utilised. For instance, the safety margins in the final compliance evaluation and the sensitivity of various factors needs to be analysed.

The first step in an attempt to go through the SKB models would be to compile a complete list of all tools that are either used directly in performance assessment or are used as a support for a particular part of the performance assessment. Documentation and quality assurance for all tools would have to be scrutinised. An effort from SKB would probably be required in order to initiate this work and finalise the documentation that is needed. The authorities also need to take additional steps to achieve a better understanding of the SKB codes, which could include various levels of engagement:

- Restricted study of code structure, including review of essential algorithms, parameters, user manuals and quality assurance procedures.
- More thorough analysis of code capability that includes running test cases and code verification.
- Extensive use of SKB codes for uncertainty or sensitivity analysis.

In addition to analysing the capabilities and weaknesses of individual codes, it is also important to obtain an overview of the integral use of codes in a performance assessment, the boundaries between various codes and the potential abstraction errors involved in transferring data between different components.

The working groups found little motivation for extensive use of SKB models in independent modelling studies, in part because both SKI and SSI already have access to codes that are similar to those used by SKB. In addition, there was some doubt as to whether or not it would be appropriate to use SKB models for regulatory review, and whether SKB's models could be relied upon to address all conceptual uncertainties that the authorities might deem important. Nevertheless, a thorough review of SKB’s quality assurance was recommended.

## 6. Needs for development of specific modelling capabilities

A series of more specialised modelling issues were identified by the working groups as being particularly important to address in the near future.

***Near-field group recommendations***

The near-field group concluded that most of the important near-field issues that are likely to arise during a review of upcoming performance assessments could be handled with existing tools and expertise. However, the group pointed to a need to develop a better understanding of coupled radiation-thermal-hydrologic-mechanical-chemical (RTHMC) processes in two subsystems:

- Coupled RTHMC processes in the canister-buffer system in a defective-canister scenario.
- Effects of radiolysis on the dissolution of spent fuel and corrosion of the canister.

General modelling capabilities for evaluating radionuclide inventory in the spent fuel, radionuclide solubilities, and radionuclide diffusion through the buffer are available if needed. SKI has devoted considerable efforts to develop tools for uncertainty analysis of radionuclide solubilities. Issues related to radionuclide transport or the stability of the barrier systems could require the use of coupled geochemistry and transport codes.

***Far-field group recommendations***

The far-field group noted that SKI has an adequate suite of modelling tools available for most questions that could arise in a review of a performance assessment. The most urgent actions were identified as:

- Early review of SKI's code requirements and capabilities regarding groundwater flow field and geochemical evolution (palaeohydrology) as this was felt to be a critical issue in evaluating site-specific safety cases and the demonstration of system understanding.
- Consolidation of the authorities' codes and capabilities for flow evolution and fracture-network flow and transport modelling.

The working group also recommended that action be taken soon to test and build SKI's experience in applying these models (especially geochemical evolution models) to site-specific data sets, and to build familiarity with the models that SKB plans to use by requesting documentation of those models and their quality-assurance status.

***Biosphere and risk evaluation group recommendations***

Significant independent modelling of the biosphere will need to be carried out by the authorities (SSI and SKI); both to develop risk-based regulatory guidelines and for review of SKB's eventual license application.

Urgent actions were identified as:

- Development of a biosphere modelling strategy document driven by regulatory needs.
- A state-of-the-art review of biosphere modelling tools,
- A review of data requirements for biosphere assessment,

This working group also highlighted needs to resolve issues regarding treatment of the geosphere-biosphere interface, to develop guidance on quality assurance for the modelling programme, and to establish an SSI/SKI working group on biosphere issues such as the biosphere/geosphere interface.

***Near-field/far-field integration group recommendations***

The working group on near-field/far-field integration issues noted that the boundary between these subsystems is not clear-cut in practice. Hence there is a need for the authorities to plan on overlapping coverage by reviewers from different scientific disciplines to ensure that interactions are properly checked.

High-priority issues identified by this group were:

- A requirement for SKB to present clear specifications regarding backfill and other repository materials, so that potential effects of the near field on far-field hydrogeochemistry can begin to be assessed.
- A requirement for SKB to give advance notice of scenarios, design parameters, and data that will be used as the basis for the safety case.

The group noted that most key near-field and far-field interactions are strongly dependent on the scenarios under consideration. Hence the above issues need to be resolved before the authorities' review capability for these interactions can be meaningfully addressed.

***Far-field/biosphere integration group recommendations***

High-priority issues identified by this group were:

- To develop a more detailed understanding of processes in the top, weathered portion of the geosphere, in quaternary deposits and between surface water aquifers.
- To develop consistent modelling interfaces between far-field and biosphere models.
- To use biosphere modelling for regulatory development, which can to a large extent be conducted independently of other subsystems.

The group felt that existing modelling tools were adequate for these purposes, but that the first issue should receive particular attention in SKB's site characterisation programme, and that the second issue requires better communication of the capabilities of far-field geosphere models.

***Review integration & strategy group recommendations***

High-priority issues identified by this group were:

- Consolidation of codes recommended by the Near-field, Far-field, and Biosphere working groups.
- Tracking of all relevant SKB reports and new information of relevance from the international literature.
- Maintaining a running list of issues for resolution with SKB via a common issue-resolution approach.

- Test and build expertise in modelling in areas identified as requiring independent modelling at the review stage.
- Review the application of SPARTA and other top-level PA codes (e.g. AMBER) for review purposes, with an eye toward developing a common framework of SKI & SSI codes for integrated assessment of the engineered barriers, natural barriers, and biosphere.
- Prepare "position papers" on state-of-the-art understanding of important issues central to the proposed SKB safety concept to act as a benchmark for issue resolution.

# 7. Conclusions

The workshop identified a set of critical issues for SKI and SSI to address in preparing for future reviews of license applications, which have subsequently been considered in preparing this synthesis.

**Structure for organising expert participation**: A structure for organising expert participation in future reviews is proposed based on clearinghouses for (1) regulatory application and context, (2) engineered barrier systems, (3) geosphere, (4) biosphere, and (5) performance assessment integration and calculations. As part of their work, these clearinghouses could identify key issues that need to be resolved prior to future reviews.

**Performance assessment strategy and review context**: Future reviews will be conducted in the context of regulations based on risk criteria; this leads to a need to review the methods used in probabilistic risk assessment, as well as the underlying process models. A plan is needed for accomplishing both aims. Despite the probabilistic framework, a need is anticipated for targeted, deterministic calculations to check particular assumptions.

**Priorities and ambition level for reviews**: SKI's and SSI's resources can be more efficiently utilised by an early review of SKB's safety case, so that if necessary the authorities can make an early start on evaluating topics that are of primary significance to the safety case. As a guide to planning for allocation of effort in future reviews, this workshop produced a preliminary ranking of technical issues, on a scale from "non-controversial" to "requiring independent modelling,"

**Analysis of repository system and scenarios:** Systems analysis tools including features/events/processes encyclopaedias, process-influence diagrams, and assessment-model flowcharts should be used as review tools, to check the processes and influences considered in SKB's analyses, and to evaluate the comprehensiveness of the scenarios that are analysed.

Aspects of the engineered-barrier design and construction methods need to be clarified by SKB so that SKI and SSI can prepare for analysing the consequences. SKB needs to have a plan for ensuring development of alternative site descriptions, and/or SKI and SSI will need to raise alternatives.

**Role of SKI/SSI models in performance assessment reviews:** An independent modelling capability will be essential to fulfil the authorities' regulatory role, as support for expert reviews and for maintaining regulatory expertise. Independent modelling (especially regarding the biosphere) is also likely to be needed to clarify the meaning of the risk-based regulations in terms of performance measures.

SKI and SSI have access to computer models covering all geoscientific disciplines and parts of the engineered barriers, geosphere, and biosphere. A review of SKI's and SSI's current modelling capability should be initiated, with an aim to check, consolidate, and document codes that are expected to be useful for future review efforts, and to develop a plan for any additional code development that may be identified as necessary.

**Role of SKB models in SKI/SSI reviews:** The working groups concluded that independent models presently available to SKI and SSI cover the main capabilities of SKB models, and hence there is little motivation to use the latter to support a review. However, the authorities will need to develop more familiarity with SKB's codes in order to obtain an understanding of the attendant uncertainties. Activities in this direction could include scrutiny of the conceptual models, documentation and quality assurance for these codes, examination of code structure and essential algorithms, or use of the codes for running test cases or uncertainty analysis.

**Needs for development of specific modelling capabilities:** The working groups identified a number of specific areas where improved model capabilities are expected to be needed for review purposes, as detailed in Section 6 of this report. The most urgent need is for a biosphere model to help define compliance criteria and provide guidance to SKB in interpreting the risk-based regulations.

## References

SKB, 1999. SR 97: Processes in the repository evolution. SKB TR-99-07, Swedish Nuclear Fuel and Waste Management Co., Stockholm.

SKB, 2001a. FUD-program 2001, Program för forskning, utveckling och demonstration av metoder för hantering och slutförvaring av kärnavfall, [in Swedish], SKB TR-01-30, Swedish Nuclear Fuel and Waste Management Co., Stockholm.

SKB, 2001b. Program för platsundersökning vid Forsmark [in Swedish], SKB R-01-42, Swedish Nuclear Fuel and Waste Management Co., Stockholm.

SKI, 2000a. SKI:s och SSI: gemensamma granskning av SKB:s Säkerhetsrapport 97. Granskningsrapport. SKI rapport 00:39, Swedish Nuclear Power Inspectorate.

SKI, 2000b.Opinions on SKB's safety assessments SR 97 and SFL 3-5: A review by SKI consultants. SKI rapport 00:47, Swedish Nuclear Power Inspectorate.

SKI, 2001. Site Characterisation – Regulatory aspects of SKB´s programme, SKI seminar November 9, 2001 Johannesbergs Slott, Sweden, Memorandum, Swedish Nuclear Power Inspectorate.

## Appendix 1: Critical issues in preparing for review of performance assessments

Ten topics related to radionuclide transport modelling were identified as critical issues for SKI and SSI in preparing for review of an eventual performance assessment.

It bears emphasising that this list of critical issues should be viewed neither as exhaustive nor permanent. The list should be reviewed continuously, and revised as necessary during the run-up to future license applications. However, this list can help to focus SKI's and SSI's preparations for future reviews, and to highlight areas in which further independent research and development by the authorities could be useful.

The critical issues identified by the workshop participants were:

- Guidance to SKB on performance measures: The meaning of the risk-based regulations in terms of performance measures needs to be clarified.

- How to interact with SKB: Guidelines need to be established for:
  - obtaining information on models that SKB intends to use
  - assessing SKB's quality-assurance procedures in terms of reproducibility, traceability, and transparency
  - ensuring access to site-characterisation data
  - assessing sufficiency of data

- Research issues: Research and modelling campaigns need to address issues central to:
  - canister longevity in the presence of defects
  - buffer performance
  - scoping climate change impacts

- Regulatory tool development: Efforts should focus on:
  - quality assurance and consolidation of codes
  - fixed versions with documentation
  - time schedule

- Review strategy: A plan should be formulated for how to make effective use of the authorities' resources in carrying out a review.

- Specification of near-field including heterogeneity of engineered barrier system: Aspects of the engineered-barrier design and construction methods need to be clarified so that SKI and SSI can make relevant preparations for analysing the consequences of the design. Real data need to be developed regarding the ability of the proposed construction methods to meet specifications including those on homogeneity of the buffer and backfill materials.

- Requirement for SKB strategy document: This should signal what SKI and SSI can expect in SKB's application regarding:
  - Safety case: How will safety be demonstrated?
  - Safety allocation: How much reliance will be placed on each barrier or barrier function?
  - Robustness of design
  - Resolution of remaining issues that have to be dealt with during the various stages of repository development
  - How will SKB resolve issues raised by SKI and SSI in their reviews?

- SKI/SSI plans for defending their decision regarding acceptance/rejection of SKB's safety case (may provide feedback to SKB strategy & vice versa)

- Biosphere model to help define compliance criteria: This is needed to provide guidance to SKB regarding the interpretation of the risk-based regulations.

- Alternative site descriptions: SKB needs to have a plan for ensuring development of alternative site descriptions, and/or SKI and SSI will need to raise alternatives. The authorities must ensure that the site characterisation strategy undertaken by SKB will provide rigorous challenges to site models.

# Appendix 2: Near-Field Group Report

**Randy Arthur**

## Group Members

Randy Arthur (Chairman)
Christian Ekberg
Pierre Glynn
Bernd Grambow
Christina Lilja
Jinsong Liu
Peter Robinson
Mike Stenhouse
Bo Strömberg
Chin-Fu Tsang

## Objective

The objective was to identify near-field issues that might need to be evaluated by SKI when a safety assessment is submitted for review and comment by SKB in support of future licensing activities for a KBS-3 repository. Of particular interest are existing gaps associated with these issues in terms of data, knowledge and modelling tools that must be filled by the time the safety assessment is submitted. Comments below are an attempt to synthesize the main points of discussion of the issues among members of the near-field group (NFG) in response to questions posed in the workshop documentation. The comments are limited to the workshop theme of radionuclide transport. The isolation function of the near field will be considered in a separate workshop. The broader issue of a general review strategy is taken up in the "Review Integration Strategy Group Report".

## PID

Figure 1 shows a simplified PID used by the NFG to focus discussion on issues that would need to be either reviewed or evaluated by independent calculations or modelling. Key near-field features (fuel, canister, buffer, backfill and near-field rock) are linked in space and time by coupled/uncoupled Radiation (R), Thermal (T), Hydraulic (H), Mechanical (M) and/or Chemical (C) processes.

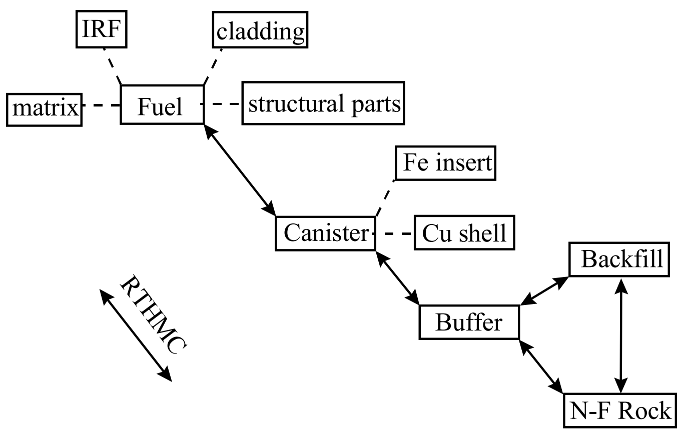


Figure 1. Near-field PID

It was considered important at this level of analysis to define the fuel in terms of its component parts, including the fuel matrix, Instant Release Fraction (IRF), cladding and structural parts. The fuel might also need to be considered in terms of type (PWR, BWR, MOX) and distribution in the repository (*e.g.,* commingled MOX and PWR/BWR fuel *vs.* disposal of MOX separately in the repository). Similarly, the canister is considered in terms of its inner cast-iron insert and the outer copper shell. Radionuclide transport is seen as the 'end-point' in an analysis of the near field, which would take the form of a "release case" calculation (see below) for radionuclide transfer to the geosphere.

## Scenarios

The next step was to identify key scenarios that could affect the near field and thus impact the simple PID shown in Fig. 1. Scenarios considered important were those that would either create new pathways for radionuclide transport, or would cause changes in the hydrogeology and/or hydrochemistry of the far field. The following scenarios were expected to be important, based on current understanding, but the NFG felt it was essential that the proponent provides notification as early as possible specifying details of repository and EBS design, and scenarios to be considered in their safety assessment:

- canister defects,
- climate change,
    - glaciation
    - uplift/erosion
    - changes in sea level
- human "mistakes", *e.g.,*
    - improper/incomplete emplacement of buffer or backfill
    - deficient sealing of shafts
    - incomplete closure
- seismic events, and
- coupled scenarios

A base scenario, in which all EBS materials function as intended and present-day conditions in the far field and biosphere extend indefinitely into the future, was not considered because the isolation function of the canister would not be compromised in this case and radionuclide transport could therefore not occur. The isolation function of the canister might be breached, however, by defects in the weld between the lid and canister body, which might escape detection during inspection for quality control. In such cases, radionuclide release from the near field would depend on defect size, defect location and the total number of defective canisters. Similarly, the EBS may not function as intended due to procedural deficiencies in emplacing the buffer/backfill, in sealing shafts and in closing the repository. The NFG felt that such "human-mistakes" scenarios had not been adequately addressed in previous safety submissions. The NFG also felt that coupled scenarios (*e.g.,* canister defect plus climate change) would be emphasized in future safety assessments.

## Review Approach

The NFG next considered how issues associated with each major component of the simple PID (Fig. 1) should be dealt with. The first step is to categorize the issues according to the anticipated level of effort needed to address them. Categories suggested in the workshop documentation were adopted by the NFG, and are summarized in Table 1. An approach that could be used to assign near-field issues to each of these categories, and to organize the effort needed to address them, is illustrated in Table. 2. As can be seen, the recommended approach would utilize individuals with expertise in radiation, thermal, hydraulic, mechanical and/or chemical processes to identify and categorize issues pertaining to each of the main components of the near field (Fig. 1).

## Near-field Issues

The NFG next exercised the approach summarized in Table 2 to identify near-field issues that are likely to remain controversial, in the sense noted in Table 1, by the time SKB next submits a safety assessment for review. Overall, the group considered that the expert judgement, scoping calculations or independent modelling required should:

- allow for strong coupling among RTHMC processes, and variations in initial and boundary conditions, [*e.g.,* oxidizing conditions resulting from 1) radiolysis, 2) residual $O_2(g)$ in the EBS and near-field rock at the time of closure, and/or 3) migration into the near-field of oxygenated glacial meltwaters in a climate-change scenario],
- permit time dependent analyses to be carried out, and
- be hierarchical in the sense that calculations could readily be undertaken at various levels of detail.

Results are summarized below for each of the near-field components identified in the simple PID shown in Fig. 1. Additional remarks are summarized for several overarching issues, including "release cases", "coupled processes" and "models and data". For each issue, the NFG's assessment of the level of effort required to address the issue is noted. All the issues discussed may require that SKI develop an *in-house* (*i.e.,* SKI staff and consultants) evaluation/modelling capability to address them, and, if so, the NFG felt that the necessary effort to develop such resources would have to be implemented as soon as possible.

Table 1. Issue categories

<table>
<tr><th>Issue category</th><th>Level of effort</th><th>Scope</th></tr>
<tr><td>Non-controversial</td><td>Minimal</td><td>Check SKB data, models and results</td></tr>
<tr><td rowspan="3">Controversial</td><td>Expert Judgement (EJ)</td><td>Detailed expert review</td></tr>
<tr><td>Scoping Calculations (SC)</td><td>Detailed expert review supported by limited scoping calculations to check SKB results</td></tr>
<tr><td>Independent Modelling (IM)</td><td>Detailed expert review informed by independent modelling of SKB data, possibly using different models and computer codes to those applied by SKB</td></tr>
</table>

Table 2. Outline of the recommended approach to identify and categorize near-field issues.

| N-F Component | Expertise | | | | |
|---|---|---|---|---|---|
| | R | T | H | M | C |
| Fuel | • | • | | | • |
| Canister | | • | • | • | • |
| Buffer | | • | • | • | • |
| Backfill | | | • | • | • |
| N-F Rock | | | • | • | • |

## Spent Fuel

There are potentially significant uncertainties in the total inventories of some radionuclides estimated using ORIGEN-type calculations, and in the distribution of nuclides among the spent fuel matrix, the gap between the fuel and cladding, grain boundaries in the matrix, and metal parts of the fuel assembly. The NFG felt that SKI should track efforts by SKB and other, international programs aimed at reducing these uncertainties to the extent possible, and to account for their effects on total radionuclide inventories and IRFs. A capability within SKI to conduct its own ORIGEN-type calculations [**SC**], or, alternatively, to conduct a thorough review of SKB's calculations [**EJ**], may be useful for this purpose.

There are major uncertainties in models of spent-fuel dissolution. The model currently used by SKB accounts for $\alpha$- and $\beta$-radiolysis of water adjacent to fuel surfaces, decomposition and recombination reactions among radiolysis reactants and products, and oxidation-assisted dissolution of the fuel matrix. The model includes significant uncertainties, however, which have not been fully evaluated by SKB. The uncertainties lie in the magnitudes of rate constants, reaction orders for oxidation reactions, the role of radicals and trace elements, and surface characteristics of the fuel matrix. The NFG felt that SKB would need to address these sources of uncertainty in future model developments, as well as recent experimental results showing that the combination of high $H_2(g)$ overpressures generated by corrosion of the canister's iron insert and a $\gamma$-radiation field strongly suppresses the dissolution rate of spent fuel. A parallel effort within SKI is needed to track progress in the modelling and experimental work, and to evaluate alternative models and data [**SC/IM**].

## Canister

The hydromechanical model developed by SKB for the canister-defect scenario suggests that radionuclide releases from the near field would not occur for 200,000 years because this is the period of time needed to develop a continuous water pathway between spent fuel and the near-field rock. The model appears to oversimplify a number of processes that are strongly coupled, however. The evolution of such systems may be sensitive to minor variations in initial states, boundary conditions, rate constants and the impact of secondary processes that were not considered in SKB's analysis. The model does not provide an adequate basis for excluding the possibility of dose exposures before 200,000 years, and SKI has therefore recommended that SKB should improve the experimental basis of their model, as well as in greater detail account for uncertainties regarding rate-determining mechanisms, uncertainties in kinetic data, the evolution of chemical conditions inside the canister, and mass-transport processes in the near field. The NFG recommended that a parallel effort by SKI is needed to evaluate model results, and to consider alternative models and data [**IM**].

## Buffer

A better understanding of the long-term chemical and mineralogical evolution of the buffer was recommended by the NFG because the chemistry of buffer porewaters will affect the mechanism and rate of spent fuel dissolution, the corrosion behavior of copper and iron components of the canister, and the solubility, speciation and sorption behavior of radionuclides. Attempts to experimentally characterize porewater compositions are complicated by ambiguities arising from the sampling techniques presently available. Models used by SKB to predict the long-term evolution of porewater chemistry are overly simplistic, are constrained solely by the results of short-term laboratory experiments, and are not fully consistent with reactions inferred from observations of natural systems containing smectitic clays. The NFG felt that SKI should track experimental, field and modelling work that can be used evaluate the reliability of SKB's proposed model of the long-term chemical and mineralogical evolution of buffer materials [**EJ**].

## Backfill

Groundwater salinities as low as 10 g/*l* have been shown to significantly reduce the swelling pressure of backfill materials, which may lead to the development of fast pathways for radionuclide transport due to imperfect sealing at the backfill-rock boundary. Engineering solutions to this potential problem are possible, including the use of different types of bentonite in the backfill mixture, increasing the proportion of bentonite to crushed rock, and/or changes in repository design. The NFG felt that if such changes in material properties or design are considered by SKB, associated impacts on safety should be assessed [**EJ**]. If it cannot be ruled out that the backfill would be more permeable than the host rock, then the hydraulic significance of tunnels would have to be assessed [**IM**]. The occurrence and possible influence of moderately saline groundwaters is an underlying factor that would have to be addressed in this context [**SC, EJ**].

## Near-field Rock

The NFG did not identify any key issues involving the near-field rock, with the possible exceptions of radionuclide transport through the EDZ [**SC**], and migration to repository depths of oxidizing glacial meltwaters in a climate-change scenario (see below). Issues that might arise involving this component of the near field due to interactions between the far field and near field are discussed in the "Far-Field/Near-Field Integration Group Report".

## Release cases

Release cases are defined by radionuclide inventories, the spent-fuel dissolution rate, solubility limiting constraints on radionuclide concentrations, and parameters characterizing the sorption of radionuclides onto buffer and backfill materials. Key uncertainties in a release calculation thus include the uncertainties in inventory and uncertainties in fuel-dissolution models, noted above, plus uncertainties that are inherent in calculating radionuclide solubility/sorption behavior. The latter uncertainties are attributable to uncertainties in the thermodynamic database used in the calculations, uncertainties in predicting the near-field geochemical environment, and/or uncertainties in the nature of solids that are assumed to be solubility limiting.

The NFG felt that the most appropriate approach for dealing with release cases and associated safety consequences was to adopt a hierarchical modelling approach. For example, a PA code such as AMBER could be used, for a given radionuclide, to assess the overall impact on release of uncertainties in the fuel-dissolution rate and the radionuclide's near-field speciation-solubility-sorption behavior. The latter uncertainties could in turn be evaluated using research-type models of coupled R-T-H-M-and/or-C processes to simulate the temporal and spatial evolution of the near-field environment, and conventional geochemical modelling software and supporting thermodynamic data to evaluate associated solubility constraints, or the impact on transport of alternative models of sorption behavior (*e.g.,* Kd *vs*. surface-complexation models). The main advantage of the hierarchical modelling approach is thus that the multiple factors and associated uncertainties potentially affecting release can be evaluated on a radionuclide-specific basis, and with specific reference to associated impacts on safety [**SC**].

## Coupled processes

The NFG felt there was a need for a "general-purpose" modelling approach and software to better handle coupled processes in the near field. An integrated model incorporating process-level models for two or more components of the near field should be developed for this purpose. Although some detail in the process models may be sacrificed to promote computational efficiency, it should be possible to adequately capture essential near-field FEPS by abstracting key results from the process models using expert judgment. An integrated model would permit a more realistic evaluation to be made of near-field conditions arising from time-dependent variations in boundary conditions at the buffer-rock, canister-buffer and fuel-canister interface. Software already used for SKI (AMBER), or other software (*e.g.,* GOLDSIM or MATLAB), may provide the basis for developing such coupled models of near-field evolution.

The NFG felt that there is presently a need to apply the general-purpose modelling approach to two systems. One is the buffer–rock system during the pre-closure and early post-closure periods of repository evolution [**IM**]. The evolution of this system will involve complex couplings among thermal transfer, hydrologic flow, chemical transformation of the buffer and rock, and mechanical deformation in the buffer and rock. Thus, because of waste heating, there will be bentonite drying and shrinkage very near to the canister. On the other hand, there will be water inflow from the rock that will increase the bentonite saturation at the outer boundary of the buffer, causing swelling with swelling pressure imposed on the rock. In some cases, the swelling pressure may be sufficient to open up rock fractures, increasing its permeability and altering the flow field around the deposition hole. In the bentonite, water flows under capillary suction and vapor predominantly migrates through diffusion, and the two phases will exchange through evaporation and condensation. At a large time into the future with the decrease of thermal output from the waste and increasing saturation of the buffer, the part of the buffer near the canister will also be saturated with water and swell. The resulting swelling pressure will be imposed on the canister. These various couplings raise a number of important questions, including:

- What is the resaturation time? That is to say, how long does it take for the water to flow from the rock, saturate the bentonite and come into contact with the waste canister?

- How will the bentonite swelling impact the integrity of the waste canister? Is the swelling pressure expected to be uniform around the canister, or is it highly uneven, with large pressures focused on a few locations on the canister surface?

- How does the bentonite swelling affect the rock around the deposition hole? Would there be a significant deformation induced on the rock fractures to change the permeability and the nearby flow field?

- What is the retention capability of the buffer for radionuclides under the changing thermal gradient and saturation profile?

The NFG felt that these questions could be addressed using existing codes, such as ROCMAS and TOUGH-FLAC, and data from recent and on-going laboratory and field experiments.

The second system is the canister-buffer system in a defective-canister scenario (see above). This model should incorporate chemical processes into the hydromechanical model developed by SKB, and should also evaluate the potential for episodic releases of gaseous radionuclides as $H_2(g)$ generated by corrosion of the iron insert is expelled out through the buffer. The NFG also felt that the effects of transient oxidizing conditions in the near field would have to be considered in a defective canister scenario. Radiolysis could generate such conditions if, for example, the overall rate of radiolytic oxidant production exceeds the corrosion rate of the iron insert. Additional potential sources of oxidants in the near field include residual $O_2(g)$ from the operational phase of the repository contained in EBS materials and the near-field rock, $O_2(aq)$ dissolved in glacial meltwaters migrating to repository depths in a climate-change scenario, and/or products of spent-fuel oxidation resulting from contact with $O_2(g)$ during storage of the fuel assemblies.

## Models and Data

The NFG felt that SKI's near-field modelling capabilities were generally adequate. It was recommended, however, that a thorough review of SKB's models should be undertaken as soon as possible. The objective of the review would be to identify gaps in modelling capabilities, which would help guide any future model development for SKI. There was also some discussion of whether SKI should consider using models developed/used by SKB. It was concluded that although SKI should in any case be thoroughly familiar with these models, and that such familiarity would be enhanced if SKI were to use the models routinely, SKI should maintain an in-house capability to develop and apply its own independent models, particularly of those near-field processes that are key to the safety case proposed by SKB.

A number of data issues may complicate application of SKI's models, however. These include:

- reliability issues (*e.g.,* should surface-complexation models and associated thermodynamic data be used to model sorption instead of the simple Kd approach?)
- data inconsistencies (*e.g.,* in experimental determinations of Kd using batch versus diffusion-cell techniques),
- data uncertainties, and the relative importance of these uncertainties in relation to scenario and model uncertainties, and
- abstraction issues (*e.g.,* can the uncertainty in an abstracted parameter value be quantified?)

The NFG felt that these issues can be adequately addressed using expert judgement [**EJ**].

## Suggested SKI Actions to Reinforce Near-Field Capabilities

The NFG concluded that most of the important near-field issues that are likely to arise during a review of SKB's upcoming safety assessments could be handled in-house using expert judgement and scoping calculations. Independent modelling may be required, however, to develop a better understanding of coupled RTHMC processes in two near-field subsystems:

- the buffer–rock system during the pre-closure and early post-closure periods of repository evolution, and

- the canister-buffer system in a defective-canister scenario

The NFG felt that the first subsystem had not been adequately dealt with in previous safety submissions from SKB. An essentially new safety function is associated with the second subsystem in SKB's most recent submission, which concludes that radionuclide releases from a defective canister cannot occur until 200,000 years post-closure. SKI has concluded that SKB's hydromechanical analysis of the evolution of this subsystem does yet not provide an adequate basis for excluding the possibility of dose exposures before 200,000 years, and the NFG agreed with this view.

Independent modelling may also be required to develop a better understanding of the effects of radiolysis on the dissolution behavior of spent fuel and on the corrosion behavior of the canister. There appears to be conflicting views at present between SKB modelers and experimentalists concerning the importance of radiolysis. This situation may in itself be sufficient reason for SKI to investigate this issue independently.

The NFG felt that SKI should carry out an early review of modeling requirements for the two key subsystems noted above, and possibly for radiolysis effects on fuel dissolution and canister corrosion. To expedite this process, it was recommended that SKI should request from SKB software that SKB has used to model these subsystems. During the next 18 months, SKI should then use the "general purpose" modeling approach noted above to develop prototype subsystem models, and develop experience in using them on appropriate experimental data sets.

# Appendix 3: Far-Field Group Report

**Neil A Chapman**

## Group Members

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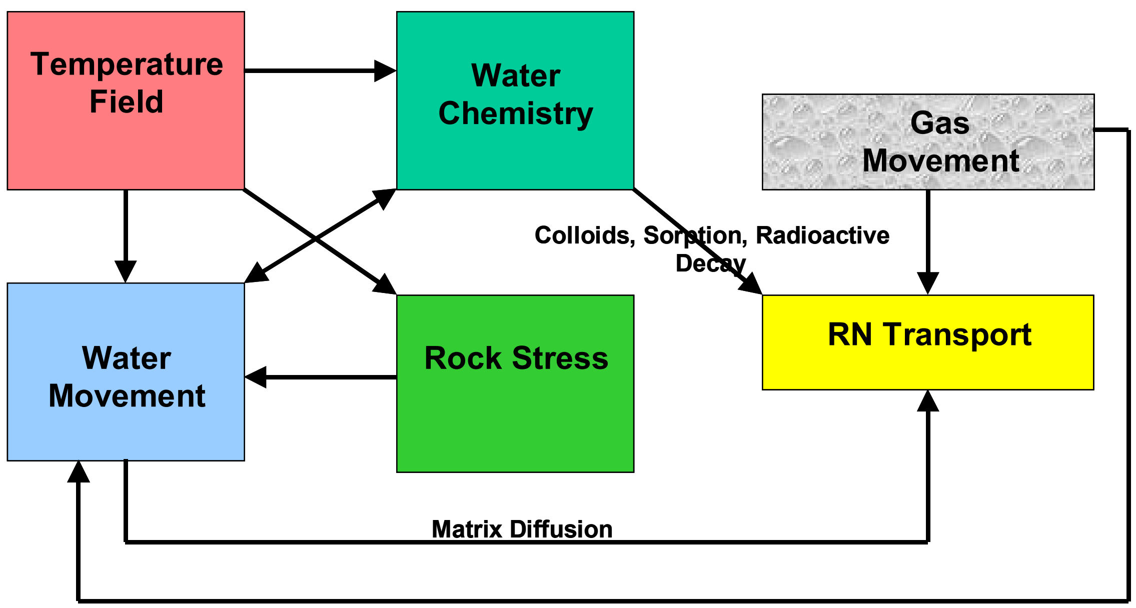
## Objective

The objective was to identify an approach for SKI to take in the hypothetical situation that it had just received a deep repository safety submission from SKB for review and comment. The aim was to use this exercise to identify key issues that might need to be evaluated, the most appropriate means of doing so, and the capabilities of SKI to mount a comprehensive review. In the process, it was intended to identify any gaps in SKI resources.

## Working with a PID

The Group addressed the questions in the manner suggested in the workshop documentation. The first task was to construct a simple PID which could be used in the working sessions to focus the thinking of the Group onto important processes/issues that would need to be either reviewed or evaluated by independent calculations or modelling. The simplest PID is shown below.



The four principal boxes in the PID are effectively equivalent to TCHM 'super-FEPs'. Some important FEPs are identified as lying along interactions between these major FEPs (e.g. matrix diffusion). Radionuclide transport is seen as an 'end-point' in analysis of the far-field, which would be in the form of an output calculation for transfer to the biosphere reviewers who would also assess radiological impacts of reference case and alternative scenario conditions.

## Scenarios

The next step was to identify key scenarios that could affect the far-field and which could impact the simple PID. The following group was defined:

- Climate change
    - ice cover sequence and cycling
    - topographic changes and erosion
    - sea coverage
- recharge changes
- Human Impacts
    - changes to water flow and chemistry (mining, waste disposal)
    - intrusion
- Deficient shaft seals
- Seismic events

## Assessing the FEPs and Assigning Review Approach

Each FEP and interaction in the simple PID was then considered, both in terms of the normal evolution of the system and in the case of scenario impacts. The objective was to assign one of the following review 'actions' to each issue identified:

| | | |
|---|---|---|
| NC | Non-controversial | Requires checking |
| EJ | Expert Judgement | Detailed expert review |
| SC | Scoping Calculations | Detailed expert review supported by limited scoping calculations to check SKB results |
| IM | Independent Modelling | Detailed expert review informed by independent modelling of SKB data, possibly using different models and computer codes to those applied SKB |

## 'Chemistry' FEP

Chemistry comprises one of the four major FEPs in the PID and effectively defines rock and groundwater geochemistry, plus the chemistry of radionuclides moving through the far-field. The major components of the FEP and the 'action' assigned to each are shown in the table below, together with the required inputs in order to be able to review each issue properly, and those that would provide essential output to groups reviewing other parts of the system. Input and output data flows concern issues that would not otherwise be treated independently by the other groups concerned.

| | | |
|---|---|---|
| Fracture surface chemistry | EJ -> IM | Input required from near-field evaluation<br>Provide output to both near-field and biosphere evaluations |
| Water composition (& Eh-pH, etc) | IM | |
| Water 'age' and evolution | IM | |
| Rock water interactions | IM | |
| Radioactive decay | NC | |
| Thermodynamic & kinetic processes | EJ | |
| Radionuclide speciation | EJ -> SC | |
| Radionuclide sorption properties | EJ/SC or IM | |

## 'Mechanics' FEP

The same approach was followed for the other Major FEPs. The rock mechanics results are tabulated below.

| | | |
|---|---|---|
| Fracture distribution & geometry (spatial variability) | IM | |
| Fracture compressibility | EJ | |
| In situ stress field | EJ | Input from biosphere (e.g. ice loading data) |
| Fracture friction/stiffness | EJ | |
| Rock strength | NC | |

## ‘Hydrogeology’ FEP

The results are tabulated below.

<table>
<tr><td>Hydraulics of major structures</td><td>IM</td><td rowspan="4">Output to near-field<br><br>(e.g. as Darcy velocity distributions)</td></tr>
<tr><td>Fracture transmissivities</td><td>IM</td></tr>
<tr><td>Hydraulic gradient</td><td>NC</td></tr>
<tr><td>Head distributions</td><td>IM</td></tr>
<tr><td>Flow-wetted surface</td><td>EJ -> SC</td><td></td></tr>
<tr><td>Recharge-discharge locations</td><td>EJ</td><td>Input from and output to biosphere</td></tr>
<tr><td>Regional boundaries</td><td>EJ</td><td>Input from biosphere</td></tr>
<tr><td>Density effects</td><td>EJ</td><td></td></tr>
</table>

## Other FEPs

The other FEPs were less complex and the actions defined are listed below.

<table>
<tr><td colspan="2">Temperature</td></tr>
<tr><td>Thermal gradient in rock</td><td>NC</td></tr>
<tr><td colspan="2">Radionuclide Transport</td></tr>
<tr><td>Matrix diffusion</td><td>SC</td></tr>
<tr><td>Colloids/microbes</td><td>EJ -> ?SC</td></tr>
</table>

## Modelling in the Review of the Far-Field

The group considered that the independent and scoping modelling requirements identified should be addressed with tools that have the following characteristics. They should:

- allow process couplings;
- allow time dependent analysis where needed;
- be hierarchical (allowing calculations to be undertaken at various levels of detail).

The main requirement for independent modelling can be seen to be in the two areas of hydrochemistry and hydrogeology (groundwater flow in fracture networks). More specifically, the Group felt that SKI would need to have capabilities to do its own modelling of:

- Water chemistry
  - composition (rock-water interaction)
  - age and evolution (palaeohydrogeology)
- Fracture flow
  - fracture network characteristics
  - time dependent flow field

These two main areas are addressed separately in the following sections.

## Water Chemistry: Rock-water Interaction Modelling

The main factors that would need to be reviewed and checked by independent modelling of SKB data were seen to be:

- redox (in particular, evidence for the presence/absence of dissolved oxygen);
- pH;
- concentration of ligands that could complex with radionuclides;
- solute concentrations (affecting groundwater density and movement).

In this area, the methodology is familiar, but will need good data sets (from SKB). It would be expected that modelling would replicate SKB results exactly. Alternative models exist for some aspects and these would need to be evaluated. An initial exercise would be to check the completeness of SKB data for each analysis and the approach of each sample to equilibrium.

In terms of code requirements and availability to carry out this modelling, SKI has access to CRACKER, EQ3/6, PHREEQE and others (e.g. Anders Worman's). SKB uses PHREEQC and M3 (Multivariate Mixing and Mass-balance), which is a tool for visualising water mixing.

Computer codes that couple the modelling of geochemical reactions to 2D/3D discretised flow models are at various stages of development internationally (e.g. UdC/Enresa in Spain have developed CORE-2D and BRGM are developing the SCS-MARTHE code that has been trialled on Äspö data). PHREEQC is now capable of 1D reaction and mass transport modelling. SKB have access only to the latter code for routine use. This area of research is likely to develop rapidly, but useful simulation of flow-mixing-reaction processes in 2D is still some way off. PHREEQC simulation of flow-reaction along single flow paths is however, possible, and CRACKER has similar capability. SKB and SKI both have capability with PHREEQC.

The databases supporting the calculations are all generic (e.g. NEA, USGS) but SKI should check SKB enhancements to recognised databases, if any. If high salinity conditions are found at any site (unlikely), SKI will need access to Pitzer approximation codes, but these are not calibrated for radionuclide chemistry so are useful only for general hydrochemistry in high ionic strength conditions. Otherwise, no problems are anticipated in addressing this general area of the review.

## Water Chemistry: Flow Evolution - Palaeohydrogeology

Modelling capabilities would be needed to undertake review in two main areas:

- forward evolution modelling of future (climate-change driven) flow patterns;
- past spatial-time stability (reconstruction of how sites achieved their present condition).

In these areas, a range of conceptual models exists. It is likely that considerable uncertainty will surround SKB interpretations. There are no widely accepted tools to model flow evolution. All the data for SKI independent modelling will come from SKB site investigations.

Modelling flow and geochemical evolution over long timescales (e.g. simulating evolution of a groundwater system with palaeohydrogeological initial/boundary conditions to the presently-observed state) is too complex for routine application. The transport-reaction codes such as CORE-2D and SCS-MARTHE can do simple transient simulations of reactive geochemistry but do not have the capability to simulate all the isotopic parameters and spatial variation. Therefore, the objective should not be complex modelling capabilities, but simple approaches that can factor in interpretations from a wide range of data types (water density, chemistry, isotopes, gases, etc). SKB have some capability for this in the DarcyTools code; another simpler approach would be to use a mixing cell approach.

SKI has no tools or experience in this important area. If it acquires them, it could test them on independent data from, for example, Sellafield, Olkiluoto, Palmottu, or Aspo. This is an area where significant effort is required.

## Chemical FEPs requiring Scoping Calculations

Both radionuclide sorption and colloid movement were considered likely to require some scoping calculations (rather than independent modelling). For sorption, SKI will need only to check the SKB data validity against accepted databases and against the water chemistry data provided (and checked independently). Although understanding of radionuclide-specific sorption will improve with time (as mechanistic models develop), it is unlikely that this knowledge will make much difference to PA data and results. If necessary, SKI can produce its own database for independent radionuclide transport calculations, based on SKB and other international data. This situation should, however, be reviewed in a few years time when there is some experience with the potential new models.

Existing transport models and codes can handle an evaluation of the potential significance of colloids. Here, a phenomenological understanding exists, but there a few if any data to validate model results. Expert judgement will be key to resolving this issue.

## Fracture Flow Modelling

Independent modelling capabilities would be needed to review:

- major structural feature models: to check whether SKB had identified a reasonable range of alternative possibilities of regional and local structure;

- alternative conceptual modelling approaches to describe groundwater flow (channel/pipe pathways, DFN, continuum): SKB should be urged to present alternative conceptual models, but SKI may wish to check the completeness/applicability of these using its own modelling of some SKB datasets;
- stress-aperture response of fractures (for seismic and climate change scenarios).

SKI should attempt to produce its own models of the groundwater flow field based on SKB data so as to understand site-specific submissions better and to be convinced that this critical aspect has been properly dealt with by SKB.

There are no problems with the availability of codes to do this. SKI uses the Geosigma MicroStation-based system for structural evaluation and has a range of flow codes to hand (Anders Worman code. FRACMAN. SUTRA and DFM). It has access to UDEC for stress and flow studies. SKB uses NAMMU, DarcyTools, CHAN3D and FracMan. SKI might want to consider the option of having access to SKB's CHAN3D code.

The main problem in this area is the resources available to SKI to carry out this aspect of the review work.

## Radionuclide Transport in the Far-Field

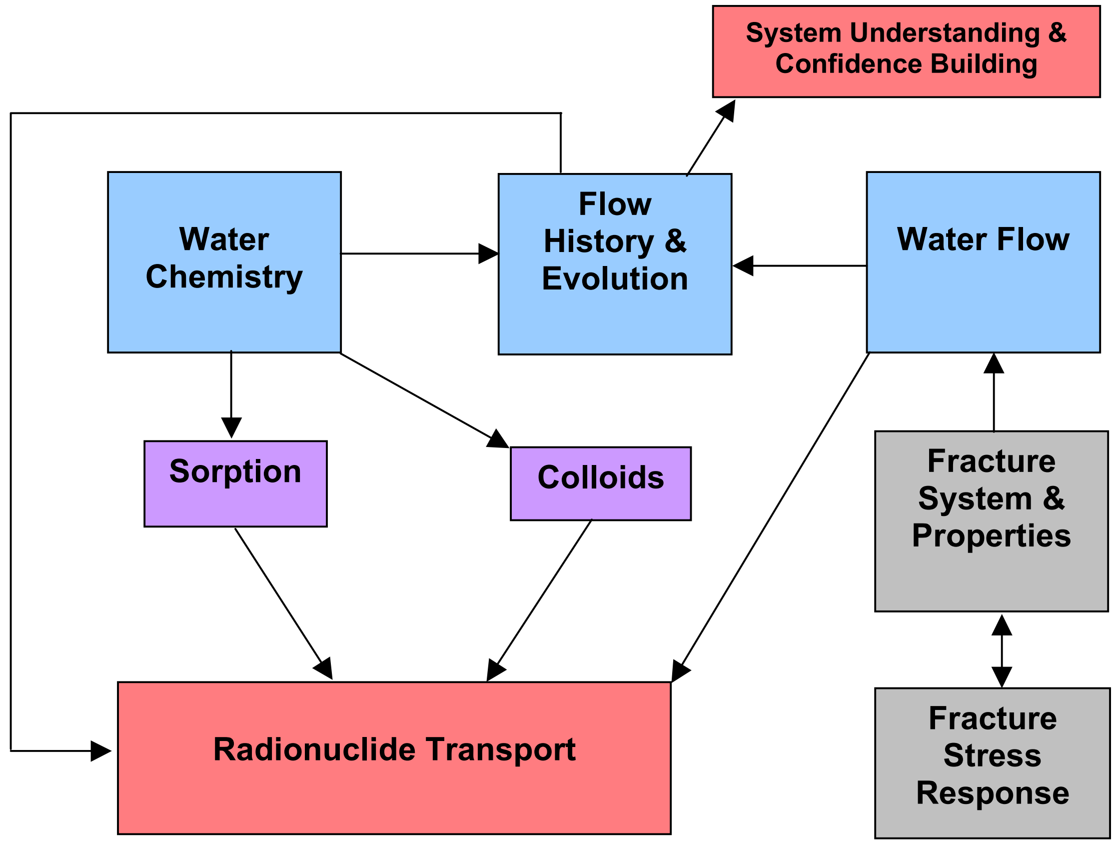
Checking of detailed transport calculations could be handled largely with the transport codes that are presently available, with the support of specialized calculations for particular 'what-if' checks. For instance, Lagrangean models may be needed to test particular assumptions that are not handled in PA compartment models, e.g. geostatistical correlations of transport and flow parameters, and abstraction errors. It is anticipated that independent comparisons of SKB's broader SA results on multiple radionuclide and radionuclide chain transport will be handled predominantly within SKI's PA codes (e.g. AMBER). Such an evaluation would use:

- a simplified flow field to produce abstracted flux data;
- sorption database;
- chemical speciation data from water chemistry modelling.

## Connection Between Far-Field Modelling Activities

The Group constructed a simple AMF (assessment model flow chart) to show the flow of information between the SKI modelling activities that would be carried out in a review. The two 'end-points' in the AMF are input to independent radionuclide transport calculations and to supporting confidence that a site is well understood.

## Suggested SKI Actions to Reinforce Far-Field Capabilities




Understanding the past and future evolution of the groundwater flow field (palaeohydrogeology) was identified as possibly the most critical support to a credible site-specific safety case. It is also the area where most uncertainty is likely to be present in an SKB submission.. Consequently, SKI has to be in a position to review this topic thoroughly. The Group felt that SKI should carry out an early review of code requirements in the two key areas of flow evolution and fracture network/flow modelling, based on the results of this brief review at the workshop. SKI should then consolidate its codes (and obtain any that are needed) for these two areas.

In the next 18 months, SKI should test and build experience in using them on site-specific data sets, especially in the groundwater evolution area.

In addition, SKI should ask SKB to provide (for all its codes) a user manual and a QA pedigree.

# Appendix 4: Risk/Biosphere Analysis Group Report

**Daniel Galson**

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## Introduction

This document summarises the discussions and conclusions of the Working Group on Risk/Biosphere Analysis. This Group was assigned a parallel set of questions to the Near-Field and Far-Field Groups. However, in addition, a question focused on risk analysis was assigned, to which the Group devoted considerable discussion. Finally, the Group, of its own accord, also addressed a broader question concerning research requirements for regulatory application. The work on the latter two questions is summarised after the discussion of biosphere issues.

The scope of the membership of this Working Group also differed from that of the other two Groups, in that it included staff from SSI.

This summary is broadly structured to follow the list of questions assigned to the Group. However, discussions did not always follow this structure; related points have been assembled under the appropriate topic for the purpose of a more coherent presentation of the Group's work.

## Principal components of the biosphere and process influence diagram

A highly simplified Process Influence Diagram (PID) for the biosphere is shown in Figure 1 (middle part, in green). The principal components are regional climate and atmosphere, regional landform and sea level, regional hydrology, soils, biota, and human interactions with the environment. The latter three are shown grouped together in the PID to simplify the Figure: they all have interactions with the regional climate and regional hydrology components of the PID, as well as with each other.

*Regional climate* encompasses the range of climatic conditions found on the relevant sub-continental spatial scales for assessment. The regional climate broadly defines the baseline characteristics of the local-scale climate, which may be perturbed from the regional norm by such factors as the location of ice-sheet margins, coastal boundaries, and anthropogenic influences. *Atmosphere* is explicitly identified to include the need to account for gaseous pathways for radionuclide exposure (inhalation).

*Regional landform and sea level* provide the upper boundary to solid parts of the biosphere system.

*Regional hydrology* includes all water bodies that form part of the biosphere component of the system, including near-surface aquifers, rivers, lakes, oceans, etc.

*Soil* includes all solid material that lies above the unweathered bedrock, and may extend to a depth of several tens of metres. It could be considered to overlap in space with the far-field geosphere.

*Human interactions with the environment* includes all of the ways in which humans may modify other components of the biosphere (e.g., irrigation, ploughing, mining, drilling).

*Biota* include all of the organisms through which human and non-human species may receive a dose by ingestion (e.g., soil organisms, crops, forests), as well as the relevant human and non-human dose receptors.

This PID includes the principal components necessary to model the biosphere at any point in time, and would likely be adequate for many applications that do not need to consider the long timescales considered for radioactive waste disposal. In addition, the PID has components for all of the major biosphere entities for which assessment endpoints might be calculated.

The PID shown at this level of detail would form a possible top-level framework for review of future performance assessments (PAs) conducted by SKB.

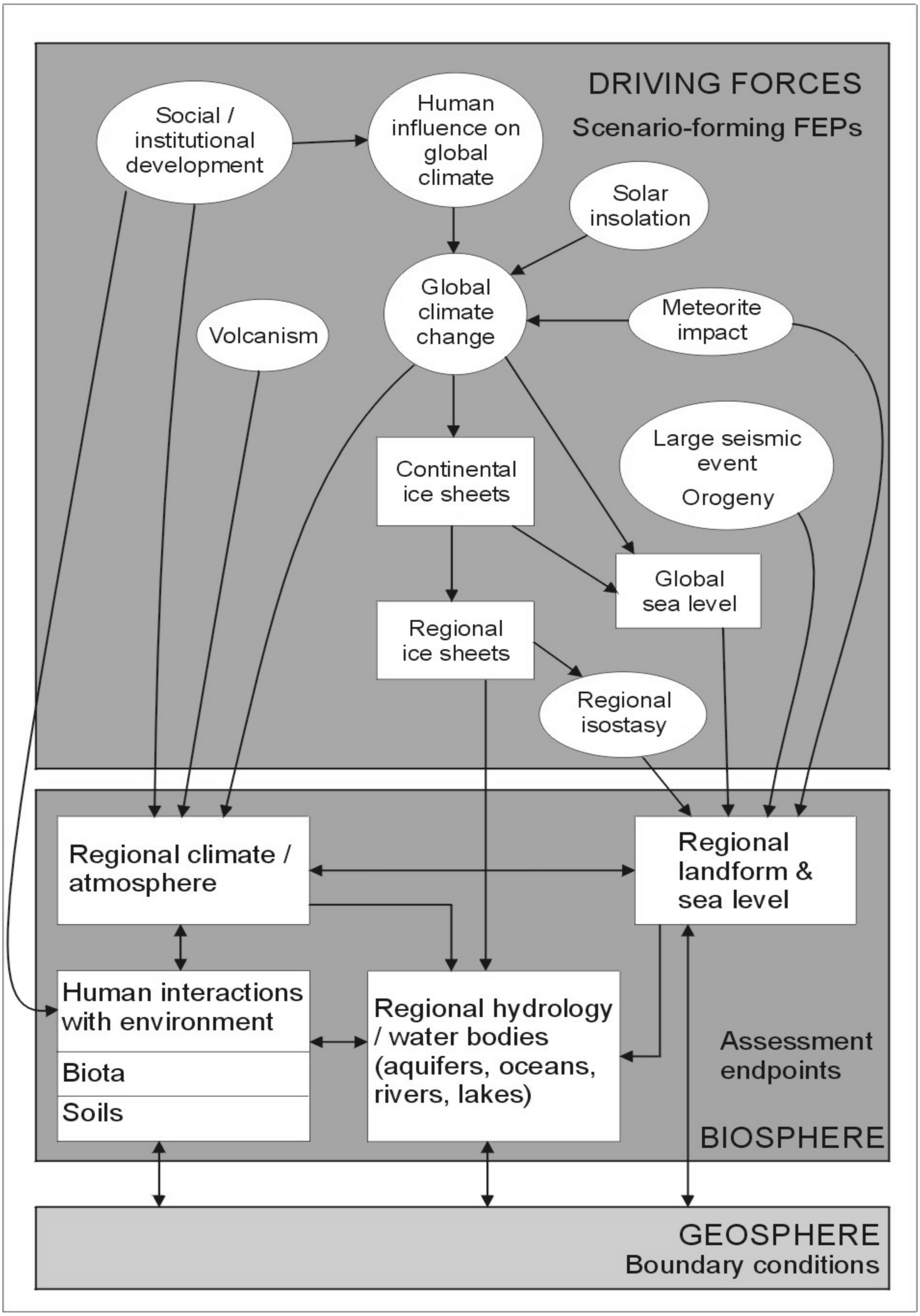


***Figure 1:*** ***Simplified PID for biosphere (middle part, in green), main scenario-forming FEPs that could influence the biosphere (upper part, in blue), and interactions with the far-field geosphere (lower part, in brown).***

## Geosphere-biosphere interface

The far-field geosphere is shown in Figure 1 (bottom part, in brown) as providing boundary conditions for the biosphere, with interactions occurring either directly or indirectly with most of the principal components of the biosphere. However, it is important to note that the location and nature of the geosphere-biosphere boundary may differ from one process to another; thus, representation of the interface as a simple boundary may not always be appropriate. Although the simplistic representation in Figure 1 provides a reasonable starting point for analysis, the Working Group participants considered that further work is required in this area, including development of a better understanding of geological, hydrogeological and geochemical processes near the geosphere-biosphere interface. The geosphere-biosphere interface is considered in further detail in the Report of the Integration Group on Far-Field/Biosphere Interactions.

## Scenario-forming FEPs

The main scenario-forming features, events and processes (FEPs) that could influence the biosphere system, and relationships between them, are also shown in Figure 1 (top part, in blue). FEPs shown in ellipses in this part of the figure are events or processes, whereas those shown in rectangular boxes (ice sheets, global sea level) are features. The scenario-forming FEPs drive system evolution, and lead to the need to consider more significant temporal changes in the biosphere, as well as temporal changes in other components of the disposal system - the driving forces shown in Figure 1 are equally applicable to the near-field and far-field. These FEPs also play a role in determining the initial conditions for modelling of the present-day system.

Occurrence of these FEPs would fundamentally influence the treatment of many components of the biosphere subsystem, as illustrated in Figure 1. For example, the development of ice sheets would affect regional hydrology and lead to changes in sea level and regional topography. Global climate change, volcanism and social developments could all significantly affect regional climate. Social or institutional development could affect the way humans interact with the environment[1].

Consideration of the possibility of human intrusion by deep drilling or mining suggests that there could be a possible coupling between the biosphere and the near-field geosphere and/or the repository itself.

Couplings between the biosphere, driving forces and the other components of the disposal system are all potentially significant, highlighting the importance of *model compatibility* between the different subsystems.

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[1] Note that consideration of social or institutional development is normally eliminated from assessments on the basis of regulatory guidance, or as being outside the assessment context However, in other work conducted for SKI and SSI specifically on the treatment of future human actions in assessments, this topic has been identified as an area where dialogue with a wide range of stakeholders could provide a firmer basis for proceeding (SKI Report 99:46 Elements of a Regulatory Strategy for the Consideration of Future Human Actions in Safety Assessments, Wilmot *et al*., 1999).

## Requirements for review and independent modelling

The Working Group participants considered that detailed review and analysis of SKB documents would be needed for all of the principal components of the biosphere subsystem, Detailed review would also be needed of SKB's treatment of the geosphere-biosphere interface and of time-dependency (e.g., treatment of climate change).

A major effort was needed on independent modelling of the biosphere subsystem for several reasons:

- To assist in the development of standards and criteria – in particular, the development of alternative performance standards to those for dose and risk. For example, "back calculations" from dose could be conducted for a specific biosphere to determine an acceptable concentration level.

- To assist with the review of SKB documents. Calculations conducted ahead of receipt of the SKB safety assessment could help prioritise the review effort, e.g., by identifying key risk drivers and areas of significant uncertainty/sensitivity. Calculations conducted as part of the review could serve to audit or check selected parts of the SKB methodology and assessment output.

- To demonstrate regulatory competence in this vital area for SSI. Biosphere calculations form a routine part of SSI's regulatory role in other areas of responsibility, e.g., emergency planning, routine releases from nuclear power stations, and SSI should be seen to be "out in front" in this area.

The independent biosphere modelling would need to give appropriate attention to the geosphere-biosphere interface, particularly for the back calculation of long-term performance measures relevant to the geosphere (e.g., turnover of radionuclides).

Independent modelling of long-term climatic effects might also be undertaken, but this was seen as a lower priority.

The new SSI regulations provide a risk-based framework for decision-making. The Working Group participants considered that a combined deterministic and probabilistic assessment approach to independent calculations may be needed. A probabilistic risk assessment (PRA) approach could be implemented for independent calculations to examine parameter uncertainty and sensitivity. On the other hand, conceptual model uncertainties and scenario uncertainties might best be considered by the regulator on the basis of "what-if" scoping calculations (i.e., probabilities need not be assigned). However, even within these scoping calculations for conceptual model and scenario uncertainty, it would be possible to consider simultaneously the impact of parameter uncertainty using a probabilistic approach.

## Biosphere model development requirements

Independent modelling of the biosphere subsystem will require the development and implementation of the following process-level models:

- Impacts on humans and on other biota.
- Detailed ecosystem-specific models.
- Transfers between ecosystems both in time (in the form of ecosystem succession) and in space.
- Climate-change impacts on ecosystems.
- The geosphere-biosphere interface.

***Approach to biosphere system model development***

Up to now, the biosphere subsystem has received little attention in independent modelling exercises that have been conducted in Sweden (e.g., SITE-94). Development and application of an independent biosphere modelling capability was identified by the Working Group as a priority topic for further work. The participants therefore identified the following as urgent needs:

- *Development of a top-level biosphere modelling strategy document*. The strategy must be seen to be driven by regulatory needs – for example, the need to conduct back calculations to establish alternative long-term performance measures.
- *Undertaking of a state-of-the-art review of subsystem model availability, capability and gaps*. The review should consider, *inter alia*, the justification, adequacy, data requirements, and strengths and weaknesses of the available models. The review should consider the current status of SSI waste management biosphere system models, biosphere models in use within other parts of SSI, developments outside of SSI in radioecology, current international projects (European Commission, International Atomic Energy Agency BIOMASS, others), and analogue information and studies, such as those conducted at contaminated sites in the former Soviet Union.
- *Assembly of a stable, well-funded SSI/SKI Working Group on the topic of biosphere modelling*. This was considered both a short-term and a long-term requirement within the programme.

The participants considered that it would not be appropriate to use SKB codes in conducting independent calculations. The regulators should place strong requirements on the quality assurance (QA) of SKB's codes. This was identified as an area where further regulatory guidance was probably needed (see below).

***Biosphere modelling issues: uncertainty, complexity, compatibility***

*Conceptual model uncertainty* should not in general be a major problem in any part of the system, in the sense that SKB will be expected as a requirement of a safety case to demonstrate adequate consideration of alternative conceptual models and related uncertainties. In addition, any independent model development and calculations will identify ahead of SKB's safety case the possible presence and importance of conceptual model uncertainty.

A number of approaches could be taken to considering conceptual model uncertainty, including parallel assessment calculations using alternative models, use of conservative assumptions where conceptual model uncertainty exists, and development of focused site characterisation activities designed to distinguish between alternative conceptual models.

The *complexity* of the models required could be expected to vary depending on the purpose of the calculation and the timescale for which the calculations were conducted. In addition, the regulatory importance of various assessment endpoints will change with assessment period. For example, the regulator will place more emphasis on dose and risk as endpoints in the first 1000 years after repository closure than at later times. Thus, models used for calculations conducted over very long periods (10,000s to 100,000s of years) could be expected to be simpler than models used for calculations conducted for relatively short periods (e.g., 10s to 100s of years). This is as true of SKB's calculations as of any independent calculations conducted by the regulators.

*Model compatibility* will be an issue particularly at the geosphere-biosphere interface. The regulators are not only facing a modelling issue here, but also an organisational issue in that SSI has in the past focused on modelling and review of the biosphere subsystem, and SKI has focused on modelling and review of the geosphere subsystem (while not excluding consideration of the biosphere).

## Biosphere data requirements

The participants considered that there was an urgent need for a data review for biosphere assessment for radioactive waste disposal in Sweden. The review would identify the availability and quality of existing data relevant to modelling of the biosphere for radioactive waste disposal in Sweden. The review was required urgently because of its importance in providing inputs to the regulators' near-term programme in the following two areas:

- Input to review of the biosphere component of SKB's site characterization programme.

- Derivation and input of parameter values for an independent biosphere modelling programme designed to establish regulatory guidance and criteria on risk assessment.

The review could take advantage of any biosphere data compilation already performed by SKB.

The review could consider the data classification framework developed within the international BIOMASS project. This system classifies data as "prescribed" (e.g., represents an international standard), generic, or site-specific. The quality of generic and site-specific data are further classified as well characterized or poorly characterized. In addition, the likely importance to calculation of various assessment endpoints is indicated.

It was considered premature to address the question of whether the site characterization planned by SKB would provide the types of data required by the regulator, as documentation of the SKB site characterization programme has not yet been completed. Any response to this question must also consider the outcome of the work to develop a regulatory modelling strategy, and the results of the state-of-the-art model review.

## Future availability of models, data and expertise

The availability of models, data and expertise into the future was considered, including methods for managing the work.

### *Management*

With regard to ensuring the availability of expertise into the future, the Working Group identified three possible management models for proceeding:

(i) A fully in-house effort, with no or only very limited use of contractors.

(ii) Retention of some in-house expertise as at present, but with a long-term contract to a "tied" technical support organisation, as in France (DSIN and IPSN) and the US (NRC and CNWRA). The support organisation would be "tied" in the sense that its ability to work for other organisations may be limited but, in exchange, there would be a long-term commitment from the regulator to provide a certain level of support. This type of system was good at minimising any perception of a conflict of interest owing to members of the contractor team working for both regulator and proponent (as is now the case).

(iii) The current *ad hoc* approach, with some in-house expertise, but short-term contracts with many contracting organisations (some of which also perform work for SKB).

The participants considered that there might be a possible half-way house between options (ii) and (iii), with some in-house expertise as at present, and a "virtual" TSO built up from several "stable" organisations having long-term contracts. This would require long-term stable funding and possibly additional in-house staff to better manage the contracting effort.

### *Data and models*

Data availability would be ensured by the regulators requiring all SKB data to be made available (from SICADA, the SKB primary database, and related SKB databases). The main issue was likely to be with the timing of data delivery, i.e., the regulators may want access to the data before it had been fully interpreted and presented by SKB.

The importance of QA of the model development process has already been mentioned. QA provides a means to build confidence in the long-term availability and usability of assessment tools, including models, codes and databases of both regulator and developer. The quality programme can also help regulators deal with the issue of model and code sustainability in two ways. First, QA should ensure adequate documentation is developed as part of the modelling programme, so that models and codes can be used by future personnel after the initial modelling personnel have left the programme. Second, it should be stipulated that ownership of any codes developed as part of the regulatory programme resides with the regulator, to ensure that future personnel are able to have access to the codes.

***Expertise***

The comment was made that, given SSI's overall regulatory role for radiological protection across all radiological issues, it should be seen to be ahead of SKB in terms of biosphere assessment capability. However, although extensive biosphere assessment experience exists elsewhere within SSI, there was still a lack of assessment experience and tools dealing specifically with the biosphere issues around radioactive waste disposal.

Additional expertise might be needed in the following areas:

- Geosphere-biosphere interface issues. Establishment of an SSI/SKI Working Group might be the appropriate way forward.

- Detailed questions concerning particular ecosystems important in the Swedish context. This expertise would probably come from within academia.

- QA procedures to guide SKB's development of assessment code and, equally, for any independent calculations conducted by the regulators. The requirements on QA for independent calculations would be particularly important where those calculations were being conducted for the purpose of establishing criteria and guidance. The necessary expertise might best come from a software house and/or from the International Standards Organisation, in addition to experience that exists within the current group of SKI/SSI consultants.

Several risk assessment issues were raised (see below). The participants considered that it could be beneficial to establish a Working Group to help develop positions on these issues; additional expertise might be needed.

Finally, the participants noted that SSI had a role to undertake independent calculations of the inventory. Independent codes for inventory calculations were not being used in Sweden, and additional expertise might need to be found to undertake calculations if a decision was made to use a different code to that being used by SKB.

## Regulatory expectations of risk assessments

The Working Group discussed several areas where guidance might be required for SKB on the conduct of risk assessments, to ensure that SKB's assessments meet regulatory expectations. Three main areas were identified where further work and development of regulatory positions was needed:

- *The development of appropriate standards and criteria for characterizing and presenting risk-based assessment outputs at different times in the future*. This development work would need to consider the form and presentation of risk measures themselves, the use of surrogate measures for risk (i.e., alternative assessment endpoints), such as concentrations in environmental media and impacts on non-human biota, and the timescale-dependence of assessment endpoints (e.g., guidance on the use of different assessment endpoints at different times in the future).

- *The development of appropriate risk assessment methodology*. A range of methodological issues were identified that might need to be considered, including the determination of parameter probability distribution functions within an iterative approach to PRA, the selection of scenarios and the treatment of scenario probability in PRA, the selection and probabilistic treatment of critical groups in PRA, convergence criteria for PRA, and the formal use of expert judgement to underpin various assumptions in a PA.

- *High-level issues associated with the conduct of risk assessments*. The high-level issues identified included the relative role of risk calculations and other lines of reasoning and argument to support decision-making on radioactive waste disposal, regulatory expectations for the treatment of human actions (and human intrusion in particular) in assessments, the use of "what-if" scoping calculations and calculations of subsystem performance, the approach to demonstrate optimisation in a risk-based regulatory framework, and the development of tools to provide traceability within an assessment and between iterative phases of an assessment.

## General requirements for regulatory application

Several high-level regulatory application issues were identified and discussed. The Working Group undertook this task because it was perceived that such overarching issues were vital to the overall success of the regulatory programme, and because of concern that they might otherwise be overlooked in the discussion and presentation of the results of the workshop.

Priority development activities include:

- Development of an approach to project management for the license application review, and for work ahead of this review, to include consideration of how contractors will be used and organised to support the regulatory work.

- Development of procedures for licensing.

- Development of a license application technical/regulatory review strategy.

- Development of an issue tracking process and system. This may need to be done cooperatively with SKB.

- Development of QA guidance to cover SKB's activities and those of the regulators more broadly.

- Development of a consultation strategy.

## Summary

Significant regulatory effort is needed for independent probabilistic modelling of the biosphere. Two primary uses of the modelling work are to help develop risk-based regulatory guidance, and to prepare for review of SKB's license application.

There is a need to assemble a stable SSI/SKI Working Group on biosphere issues. Funding, particularly for SSI, may need to be increased in order to put in place a viable work programme. Urgently required actions include development of the following:

- A biosphere modelling strategy document driven by regulatory needs.
- A state-of-the-art review of biosphere model availability, capability and gaps, ahead of any further development of independent modelling tools.
- A review of data requirements for biosphere assessment for radioactive waste disposal in Sweden, as input to review of SKB's site characterization programme and the regulators' independent modelling work.
- Development of guidance on QA for the modelling programme.
- Work to resolve issues associated with the treatment of the geosphere-biosphere interface in assessments.

Early thinking and work on the conduct of risk assessments that can meet regulatory expectations is also urgently needed.

In the slightly longer term, there are several broader regulatory development activities that need to be established in support of regulatory application.

# Appendix 5: Review Integration Strategy Group Report

**Neil A Chapman**

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## Objective

The objective was to consider a possible structure for the review process that made best use of the resources available to SKI and SSI. The existing tools and databases for the application of a systems approach were reviewed for possible use. The immediate steps that might be taken to prepare for an upcoming review were proposed.

## Structuring a Review Using the Systems Approach

The Group considered that the Clearing House (CH) approach to concentrating expertise would be the best way of making efficient use of the resources available. It would provide the best value to SKI-SSI from their experts if they were to work together on a common set of issues. It could be used as a basis for organising work from now onwards: that is, in both the run up to a review and then in the review itself.

Six CHs were proposed:

- Inside Canister (fuel and insert) INCAN
- Outside Canister (canister degradation and buffer) OUTCAN
- Flow-Field (stability and evolution) FLOW
- Biosphere BIOS
- PA Integration & Calculations (SA calculations) PAIC
- Regulatory Application & Context RAC

The existing tools to manage a systems approach such as developed by SKI in SITE-94 and subsequently are:

- PID-AMF methodology, which this workshop had shown could be usefully applied at even a coarse level to focus thinking;
- FEP encyclopaedia, which is still to be published and which the Group felt ought urgently to be made available;

- SKB Processes Report from SR 97, which covers some of the same ground as the FEP encyclopaedia;
- SPARTA code for managing PIDs and AMFs;
- AMBER, and other codes, such as ECOLEGO, for PA calculations.

One of the first tasks of the **PAIC** would be to carry out the code consolidation recommended by the three previous working groups. It should also review the application of the existing tools, SPARTA, AMBER, ECOLEGO (etc) to decide whether they are sufficient for its own purposes or would need to be replaced, updated or supplemented with other codes. The objective would be to develop a common framework of compatible SKI and SSI codes that can be used for an integrated assessment of radionuclide transport in the engineered and natural barriers, as well as the biosphere. The PAIC would act as the 'master CH' by centralising and co-ordinating the activities of the four region-specific CHs (INCAN, OUTCAN, FLOW & BIOS). As work progressed, and particularly during the review itself, it would co-ordinate the use and the transfer of information. It could also formulate a common 'issue resolution' methodology for use by SKI-SSI from this point onwards. This would be a formal system of recording issues and discussions, and how they were resolved with SKB.

The **RAC** would have the task of addressing matters of regulatory policy, some of which need thinking about now. In this context, it is important to build an organisational CH structure that facilitates development of an integrated view on risk assessment, analysis of the geosphere-biosphere interface and other areas of common interest to SKI and SSI. Examples of the topics the RAC could consider are how:

- the licensing processes at SKI and SSI will interlock
- interactions with SKB would take place in the run-up to submission and in the review period;
- to address and react to uncertainties and ranges in SKB's quantitative SA results;
- they want to see scenario likelihood presented within the risk framework;
- they will weight scenarios that produce elevated doses when reaching decisions;
- to define the right stage in the SKB programme to resolve the human intrusion issue;
- to utilise comparisons of releases with natural radioactivity;
- to define compliance;
- to deal with the site SA inter-comparison ('safest site') issue;
- SKI-SSI will present their decision-basis to the public, both in a transparent ongoing fashion over the run-up period, and when a license decision is eventually required.

## Common CH Activities in Run-Up Period (next 2-3 years)

The following activities could form the basis for each CH to organise its work:

- Review and consolidation of codes and models (co-ordinated by PAIC);
- Tracking all relevant SKB reports and being fully conversant with them;
- Circulate new information of relevance from the international literature;
- Revisit the results of this workshop to check and refine the key issues identified;

- Maintain a running list of issues for resolution with SKB via the common issue resolution approach;
- Carry out test (and 'expertise building') modelling in critical areas identified at this workshop which would require independent modelling at the review stage;
- Prepare position papers ('white papers') on state-of-the-art understanding of important issues central to the proposed SKB safety concept to act as a benchmark for issue resolution. These would be considerably more in-depth than the SKB Processes or SKI FEP encyclopaedia and would be expected to define the regulators' current position and requirements on that issue.

Some further general observations were made by the Group:

- It will be important to co-ordinate these activities with those of SKI's INSITE project, and SSI's corresponding OVERSITE project, tracking the SKB site investigation work.

- Some arrangement needs to reached soon with SKB for access to information at an unpublished (or informal SKB report) stage: for example, the most recent repository design.

- The structure, working pattern, terms of reference and membership of the CHs needs to be arranged soon, if SKI-SSI decide to proceed with the approach suggested by the Group.

# Appendix 6: Far-Field/Biosphere Interactions Group Report

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## Review of the biosphere PID

The process influence diagram (PID) shown on page 39 in this report was examined. No further interactions were identified.

The participants noted that both the geosphere and biosphere were three-phase systems, consisting of rock (or soil), fluid and gas. Radionuclides could be transported across the geosphere-biosphere interface in all three phases. Solid and fluid components of the biosphere system also had the potential to influence the geosphere. There was a need for an integrated view of the two systems. A detailed study of the upper several tens of metres of the weathered rock could help support the building-up of a coherent and consistent model of this part of the system.

External driving forces (particularly climate change) were seen as providing boundary conditions in time and space for the assessment of both biosphere and geosphere performance. The need for a consistent spatial and temporal treatment of climate-change effects for the biosphere and geosphere was emphasized. The biosphere system itself also provided necessary boundary conditions for an evaluation of geosphere performance. For example, sea level and the form of the topography were necessary inputs/boundary conditions to hydrological modelling of the geosphere.

## Prioritization of geosphere-biosphere system components in model development

The interactions were conceptualized in terms of fluid transport, solid transport, and gas transport. A four-fold prioritization was developed:

(1) Must be considered in modelling of the geosphere-biosphere interface.

(2) May need to be considered in scoping calculations.

(3) Likely to be unimportant in modelling of the geosphere-biosphere interface.

N/A Not applicable.

The interactions were then prioritized as shown in the following table:

| Effect<br>Transport Phase | Hydrological effects (time, space) | Radionuclide transfers (time, space) | Colloids (organic, inorganic) |
|---|---|---|---|
| Fluid | 1 | 1 | N/A |
| Solid | N/A | 1-2 | 2-3 |
| Gas | N/A | 2 | N/A |

The Group emphasized the need to consider both the spatial variability and time dependence of the interactions.

## Key parameters characterizing the geosphere-biosphere interface

The key parameters that characterize the priority-one interactions are shown in the following table:

| Effect<br>Transport Phase | Hydrological effects (time, space) | Radionuclide transfers (time, space) | Colloids (organic, inorganic) |
|---|---|---|---|
| Fluid | Flux/area, time, spatial domain | Concentration, extent (point, distributed), time, spatial domain | N/A |
| Solid | N/A | Concentration, extent (point, distributed), time, spatial domain | 2-3 |
| Gas | N/A | 2 | N/A |

Boundary conditions are also key parameters, and these conditions need to account for climate-change effects.

## Adequacy of data and models to describe the geosphere-biosphere interface

With regard to data, the need was identified to develop a more detailed representation of the top approximately 100 m of weathered rock. This zone should receive particular attention in SKB's site characterization programme. Currently available modelling tools were considered to be adequate to represent this zone.

There is also a current need to use biosphere modelling for regulatory development. Such biosphere modelling can be conducted largely independently of the modelling of other subsystems, such as the geosphere. Tools that are fit for purpose are likely to be currently available (but see the conclusions of the Working Group on Risk/Biosphere Analysis). However, the biosphere models must be constrained by an understanding of the geosphere, and what can be or will be calculated as the output of geosphere assessment models, particularly if biosphere modelling is used to back calculate acceptable risk-based concentrations of radionuclides in the far-field geosphere for use as long-term performance criteria.

# Appendix 7: Far-Field/Near-Field Integration Group Report

**Joel Geier**

## Group Members

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| Christian Ekberg | Fritz Kautsky |
| Allan Emrén | Christina Lilja |
| Pierre Glynn | Jingsong Liu |
| Bernd Grambow | Yvonne Tsang |

## Objective

The objective for this working group was to identify the main interactions between near-field and far-field subsystems of a KBS-3 type deep repository, and to recommend an approach for SKI to take in assessing these interactions in the course of reviewing a safety case from SKB.

## Main Interactions

The group considered couplings/interactions that had been identified between the near-field and far-field subsystems, and whether additional interactions could be identified. Based on this discussion the following main interactions were identified:

*Far-field effects on near-field chemistry:*
- Groundwater evolution.
- Climate evolution (e.g. oxygenated glacial meltwaters).
- Effects of repository on hydrology (e.g. upconing of brines).

*Near-field effects on far-field chemistry:*
- Concrete and organic materials left in tunnels (affects solubilities, sorption coefficients).
- Buffer reactions.
- Backfill reactions (including crushed rock in backfill, if used).

*Far-field effects on near-field hydrology:*
- Groundwater flow to near field.

*Near-field effects on far-field hydrology and radionuclide transport:*
- Colloid generation from bentonite.
- Hydrogeochemical effects of repository operations on fracture minerals (e.g. temperature, pressure changes affecting calcite dissolution/precipitation in fractures).

*Far-field rock mechanical effects on near-field:*
- Fault activation (e.g. in response to glacial loading/unloading).
- Coupled scenarios involving fault activation in combination with variable saturation of buffer (tilted canister) or canister defect.

In addition to these near-field/far-field interactions, the group noted that there could be important interactions between different parts of the near-field system, some parts of which might be regarded as parts of the "far-field" depending on the context in the safety assessment. A broad definition of the near field as "any part of the system affected by repository operations" might not correspond to the practical subdivisions that are realised in representing the repository system by different component models.

Considering this, the group suggested that attention should be given to the influences of the tunnel system, backfill and seals on:

- Near-field hydrology.
- Near-field groundwater chemistry.

as important interactions within the near-field subsystem.

## Key Parameters

The main parameter characterising hydrologic interaction between the near-field and far-field subsystems is groundwater flux. The group agreed that evaluation of this parameter based on site hydrology models is straightforward, provided that these models contain an adequate representation of the heterogeneity.

Effects of far-field chemistry on the buffer are sensitive to the presence of deep brines or seawater. The key parameters are calcium and chloride concentrations in the case of deep brines, and potassium and magnesium concentrations in the case of seawater.

[Did we overlook effects of oxygenated waters on the canister and parameters that would relate to this?]

Chemical effects of the near field on the far field were judged to be largely a function of repository design parameters which need to be clarified. For example, the repository could give rise to a high-pH plume depending on the amount of concrete that is left in the repository. Whilst the KBS-3 design concept does not explicitly include use of concrete except in tunnel seals, the group raised the possibility that concrete could be used for other practical purposes during construction, such as for equipment pads or shotcrete for stability.

The group noted that the details of backfill specifications must be known in order to assess the potential chemical effects on far-field chemistry. The mineralogy and chemistry of the backfill, including crushed rock (if used) and organic materials (if left as artefacts of the construction), will need to be assessed. If crushed rock is used, the degree of fragmentation will affect the available surface area for rock-water interactions. The time that the crushed rock is exposed to the atmosphere between crushing and emplacement could also influence its effect on chemistry.

## Level of Analysis

The consensus of the group was that the interfaces between components of the near-field and far-field subsystems were in most cases straightforward. The group recommended a combination of expert judgement and scoping calculations to review interactions regarding:

- Chemical processes
- Colloid generation
- Groundwater evolution
- Variable resaturation of the buffer and the consequences of uneven swelling pressure for canister failure in an earthquake scenario

The most significant need was agreed to be **more data** on which to base scoping calculations, **rather than** development of **models** to assess these interactions. Ensuring that adequate data are obtained from site characterisations and accessible to the review team, including data on repository materials, is thus the key considerations.

The group noted that most key near-field/far-field interactions are strongly dependent on the scenario. This means that, in a review, these interactions should be considered primarily in the context of specific scenarios in which they are most likely to be significant. As a corollary, a review of the significance of a particular interaction may not be meaningful if this is done only for a base scenario.

## Key Needs

The following points were identified as key needs and issues to be dealt with as SKI and SSI prepare for an eventual review of a safety case.

First, it is recognised that the boundary between near-field and far-field subsystems is not clearly defined, and care must be taken that important interactions are not overlooked as a consequence. Hence the group recommended that a review should allow for overlapping coverage by reviewers from different disciplines, to ensure that adequate coverage is given to interactions among components corresponding to different scientific specialities.

Second, to allow for adequate and timely review, the safety-case proponent should be required give advance notice of the scenarios, design parameters, and data that will be used as the basis of the safety case.

Finally, the proponent should be required to present clear specifications regarding backfill and repository materials, including the degree to which materials such as concrete will be used, to remove a major obstacle to scoping the effects of these materials on near-field and far-field chemistry.

## Appendix 8: List of participants

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## Appendix 9: Extended Abstracts

# Radionuclide transport modelling: Current status and future needs

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The purpose of the seminar is to summarise the present status of relevant SKI projects and to generate a plan of actions needed for the preparation of reviewing future performance assessment (PA) submissions. A reasonable period of consideration should be 4-5 years, which has been selected based on the current SKB planning. The seminar will hopefully provide a context and a basis for new activities that need to replace some of the R&D projects that have recently been finalised or are about to be finalised.

The SKI R&D programme has for many years focussed on supporting independent research in critical areas and development of competence relevant in the PA context. However, since the Swedish programme is now approaching an implementation phase, it is necessary to change the priorities. A larger emphasis needs to be placed on utilising what SKI has previously developed and focus more closely on SKB's ongoing activities. SKI's and SSI's review of SR97 (SKI report 00:49), supported by in-depth expert reviews (SKI report 00:37), provides a good starting point for assessing SKB's viewpoints and priorities. Since some of the background information that are likely to be used in SKB's future performance assessment work are already available, it is possible to already now start the preparations for future review efforts.

The title of the workshop ("radionuclide transport modelling") should be interpreted in a rather broad sense including necessary subjects needed for RN transport modelling, such as the source term, groundwater flow, biosphere exposure pathways. The seminar should not address the assessment of barrier degradation (e.g. copper corrosion), since this will be a topic of an SKI initiative in the near future. Site characterisation issues will be discussed separately the day after the seminar but issues related to how to use data obtained from site characterisation might have to be touched upon. In addition to the technical and scientific issues, some limited efforts could be devoted to consideration of review methodologies.

In order to have an efficient dialogue about technical issues; most of the work will be done in three working groups:

- Near-field issues
- Far-field issues
- Biosphere and risk evaluation issues.

The groups will during their first session discuss general PA issues based on a list of suggested topics. The second session should be devoted to more specialised model-specific issues. A third session will deal with integration of the above mentioned topics and how models and data need to be coupled. The major findings of the three working groups will be discussed at the closing plenary session. A synthesis of this discussion will form the basis of a status report from the seminar that, if appropriate, will be published in SKI's report series.

An important and now widely accepted tool for developing a performance assessment is the system analysis, which in the end should provide a demonstration of that the performance assessment covers all relevant features, events and processes (FEPs). In reviewing a safety assessment, there is a corresponding need to ensure that all relevant aspects have been looked at in an appropriate level of detail and that there is a communication and transfer of information between those looking at neighbouring parts of the performance assessment. However, since SKI and SSI have limited resources and personnel available, there is a need for a form of very simplified PID that would only be used to organise the review. The workgroups are therefore asked to split up their theme in different parts/topics and show how the parts/topics are connected. The number of parts that can be handled effectively for each workgroup is perhaps 5-10. Each part would not necessarily be composed on a FEP or a group of FEPs but rather any kind of unit defined only for dividing the topic in a logical way.

The level of regulatory scrutiny directed to a particular part of the performance assessment should be affected by how much the representation of that part affects the final outcome of the analysis. All the different parts of a PA will, depending partly on the proponent's safety allocation priorities, not be equally sensitive. It is also natural that a larger emphasis is placed on parts of the PA where the representation is a subject of scientific controversy. Additional consideration can also be made, e.g. that events that may contribute to early releases of radionuclides should be more cautiously judged than those that could only do so in very long time perspectives. The working groups should based on their experience (e.g. from SITE-94, review of SR97), attempt to provide some kind of ranking with regard to the different parts of the PA (e.g. indicate areas where a lower level of scrutiny might be needed).

The safety allocation utilised in SR97 suggests that reliance on radionuclide retardation is given a rather limited role in the overall performance assessment. Instead, a larger emphasis is placed on radionuclide isolation, the slow degradation of any defective canisters and slow fuel corrosion. In relation to these SKB priorities, the SKI project portfolio appears to have a stronger emphasis on radionuclide transport modelling, and a good argument for this is that RN transport models must have a key role in compliance evaluation and may be the part of the PA that require the largest and most comprehensive quantitative framework. Nevertheless, it is still important that an attempt is made not only to suggest additional activities but also to suggest areas where the present SKI affiliated competence in the area of RN transport appears to be sufficient for future review purposes.

One can distinguish different activities in the preparations for reviewing a performance assessment, which represent different ambition levels, contain different proportions of independent modelling and different allocations of resources, e.g.: 1) use of expert judgement to establish a regulatory viewpoint, 2) use of scoping calculations to evaluate the reasonableness of intermediate results, 3) use of a constrained independent PA, which includes an in-depth analysis of a selected group of processes, and 4) a complete independent PA to corroborate the proponent's results and explore conceptual uncertainties. SKI's and SSI's review of SR97 included the activities within the first and in a few cases the second category described above. However, no systematic and independent corroboration of SKB's key results was considered necessary at that specific stage of repository development. A partly relevant comparison could be made with SKI's own performance assessment project SITE-94, but the focus of the latter project was rather different since the main objective was development of PA competence.

In the future preparations for new safety assessment submissions, we expect that activities within the above mentioned categories 1)-3) will be needed. The development of a complete independent PA will probably be too resource demanding and might even be inappropriate since it may divert attention from the proponent's PA. At the lowest ambition level, it may not be possible to resolve and prioritise the concerns encountered while conducting the review. This means that also a problem that may turn out to be minor ones has to be pointed out in the review. Based on these considerations, the working group members should try to justify why a particular ambition level will be needed to address a particular issue. The potential uses of existing modelling tools judged to be relevant should be suggested. Additional model development and refinement of existing models can also be suggested, but the limited resources and timeframes needs to be considered for these cases.

In order to limit the often very resource-demanding development and uses of modelling tools, it is essential that the modeller/reviewer has a clear idea about how modelling results can be used to support the review. Independent models could e.g. be used to confirm SKB results, analyse parameter sensitivity, explore simplifying assumptions, and analyse safety allocation. Once the objective with a particular use is clarified, it is also important to assess whether or not the activity is connected to other parts of the review. For instance, could a study of parameter sensitivity give guidance for those evaluating the experimental basis for the proponent's data selection, or could the model results be useful in setting up an independent PA-level model.

An alternative or complement to developing alternative modelling capability might be to focus on using the proponent's modelling tools. This might be a cost-effective way of understanding modelling results and obtaining confidence that QA measures implemented by the proponent is sufficient. The proponent's models could be used for ranking the importance of different parameters (uncertainty and sensitivity analysis) and guide the level of scrutiny needed in reviewing measurement accuracy and parameter abstraction schemes. However, it would probably not give the same level of scientific understanding, as one would receive in constructing an alternative model. The work group members could suggest different uses of the proponent's modelling tools as an alternative to using or developing independent models.

There might be areas where the expertise within SKI and SSI at its associated consultants and researcher need to be complemented with expert views from narrow scientific disciplines. One way of achieving these expert views would be to appoint a group composed of experts associated on an ad-hoc basis. SKI consultants and researcher could still be part of such a group in order to convey the performance assessment context. The work group members should indicate whether or not there any topics that might be suitable to address in this way.

Finally, it is instrumental that all the tools and data discussed above are readily available at the time of a performance assessment submission. There is no guarantee that all the individuals participating in SKI or SSI development work are available at the time of a major review. The work group member should therefore think about actions that could be taken to ensure that models and data more available and reasonably easy to use at the time of an in-depth review.

# SKB's approach for RN transport modelling and related issues

Patrik Sellin, Jan-Olof Selroos, Ulrik Kautsky and Allan Hedin, SKB

## 1. Introduction

This paper summarises SKB's achievements in fields related to radionuclide transport modelling after the completion of SR 97 [1] as well as future plans in the area. Issues identified in the SR 97 study as well as in the reviews of the report [2], [3] form the background for the development programme which is presented in SKB's RD&D programme 2001 [4].

## 2. Calculation methodology

Since the completion of SR 97, SKB has, in what may be collectively termed calculation methodology accomplished the following:

<u>Analytical models</u>: Analytical approximations to the numerical near field and far field radionuclide transport models have been developed [5]. The agreement with numerical models is good for the calculation cases considered in SR 97. Also the probabilistic calculations have been repeated with similar results.

<u>Extended probabilistic calculations</u>: The analytical models were used to extend the probabilistic calculations in SR 97. A number of findings with the potential to simplify future calculations for this system emerged [4], [6]:

- The calculation results are rather insensitive to assumptions regarding details of input distributions as long as the mean and the variance of the distributions are fixed.
- several correlations between input distributions, which can be expected from the understanding of the system, have been shown to be of minor importance for the calculation results.
- The probabilistic results of SR 97 are totally dominated by Ra-226 directly released from the canister if the rock retention is poor, and by the instantaneously accessible fraction of I-129 otherwise.

Furthermore, several of the probabilistic results from the hydrological calculations in SR 97 have been propagated to probabilistic transport calculations to further elucidate the importance of uncertainties in the hydrological analyses.

<u>Methods for sensitivity analysis</u>: The simplified approach to sensitivity analysis used in SR 97 has been complemented with more sophisticated and established techniques [6]. These include rank order correlations, linear regression on logarithmic values, and a tailor made regression model obtained from insights gained with the analytical models.

SKBs future plans in the area of calculation methodology are briefly outlined in RD&D programme 2001 [4] and will be further detailed together with other aspects of PA methodology in a methodology report planned for 2002. The report will cover e g scenario development and role of probabilistic calculations including choice of method for determination of input distributions.

## 3. Near field issues

In SR 97 and its reviews, a number of areas were identified where additional research or model development are needed. Below, a few of those areas are mentioned. More detailed plans are presented in [4].

- The spent fuel alteration model used in SR 97 has some drawbacks. Presently, the most realistic alternative seems to be an $UO_2$-solubilty limited model, based on the assumption of catalytic activation of hydrogen at the fuel surface.

- The very reducing conditions in a defective canister could mean that the trivalent state is the dominating for plutonium. The database for Pu(III) solid phases is very limited and this will be studied in the current research programme.

- SR 97 identified some shortcomings in the database for radionuclide half-lives. This database will be reviewed and quality controlled well in time before the next safety assessment.

- Since SR 97, it has been found that organic colloids have about the same diffusivity in bentonite as anions. At higher ionic strength their diffusivity is even higher, which is surprising. The studies of colloid transport through bentonite will continue.

- There will be additional development of the model for near-field geochemistry. The model will be tested with the vast amount of data available.

- The conceptual model for the mass-transfer between buffer and rock will be developed. The current model assumes a very simplified geometry.

- The general performance of the backfill was identified as a prioritised research area in SR 97. This will include choice of backfill materials and backfilling technique, long term performance of the backfill as well as a study of the backfill as a transport path for radionuclides.

## 4. Far field flow and transport

In SR 97 the groundwater flow model HYDRASTAR was used for calculations on the site-scale whereas the models NAMMU and PHOENICS were used on the regional scales. A number of limitations were identified with HYDRASTAR; for future PA analysis, the models NAMMU and DarcyTools (formerly called PHOENICS) will be used on both the regional and local scales. Development and testing of the two models are currently being performed in order to obtain all the desired features/functions.

The development programme for NAMMU shows that embedded grids (nested models) with stochastic generation of permeability fields on both the regional and local scales are feasible [7]. Also, stochastic, transient simulations including salinity driven flow and using nested model scales are feasible [8]. The development of DarcyTools has so far emphasised generation of continuum conductivity fields based on discrete fracture data [9,10,11,12]. However, nesting of model scales is currently also being investigated [13]. Both NAMMU and DarcyTools are to be fully operational including all desired features/functions in time for the site characterisation phase. Remaining work is mainly related to nesting of discrete fracture network models within the continuum site-scale models.

Radionuclide transport in the geosphere was modelled with the tool FARF31 in SR 97. FARF31 will be used for future analyses as well; however, the model will be compared to more complex process models. Furthermore, the model will be restructured such that estimates of the transport resistance (F-factor) obtained from primarily discrete fracture network models can be used directly as input for the model.

## 5. Biosphere

SKB's biosphere program [4] considers the understanding and description of the processes important for radionuclide transport and exposure in the biosphere as well as the development of necessary numerical tools. The numerical tools (BIOPATH and PRISM) have been used since the 80´s and need upgrading to modern platforms allowing efficient input of site specific data from e g GIS systems. During the next period, upgrading or replacement of the tools will be considered. The new tools should support a systems ecological approach. Moreover the tools need to support the calculation of risk as required from SSI, however more precise definitions from SSI are needed for a correct interpretation.

The documentation of important processes will continue with the refinement of the biosphere matrix. The development of the systems ecological approach has yielded promising results and will be continued and intensified. The advantages with the approach are that general transport mechanisms are distinguished from radionuclide specific transport. This gives scalable models for different sites and future ecosystems and allows assessments of radionuclides where limited knowledge is available about e g accumulation factors. Moreover, the site-specific data collected in the siting programme can directly be used in the modelling. The approach considers all pathways and compartments in the ecosystem, which is necessary when the effect on the environment should be considered according the regulations from SSI.

Special studies will consider processes in wetlands, forest ecosystems and sediments. The interface between the geosphere and biosphere also needs further studies.

## 6. References

1. Deep repository for spent nuclear fuel. SR 97 – Post-closure safety, Volumes I and II, SKB TR-99-06, Svensk Kärnbränslehantering AB, 1999

2. SKI's and SSI's Joint Review of SKB's Safety Assessment Report, SR 97 Summary, SKI Report 01:3, SSI Report 2001:02

3. SR 97: Post-closure safety of a deep repository for spent nuclear fuel in Sweden. An international peer review, Nuclear Energy Agency. Organisation for Economic Co-operation and Development, 2000

4. RD&D programme 2001. SKB TR-01-30, Svensk Kärnbränslehantering AB, to be published in English December 2001.

5. Hedin, A; Integrated Analytic Radionuclide Transport Model for a KBS 3 Repository; Accepted for publication in Nuclear Technology.

6. Hedin, A; Probabilistic Dose Calculations and Sensitivity Analyses Using Analytic Models; Accepted for publication in Reliability Engineering and System Safety 2001.

7. Marsic, N., Hartley, L., Jackson, P., Poole, M., and Morvik, A; Development of Hydrogeological Modelling Tools Based on NAMMU, SKB R-01-49, 2001a.

8. Marsic, N., Hartley, L., Sanchez-Friera, P., and Morvik, A; An Embedded Regional/Local-Scale NAMMU Model of Natural Transients in Saline Groundwater Flow: An Illustration using the Beberg Site, SKB R-01-50, 2001b.

9. Svensson, U; Representation of fracture networks as grid cell conductivities, SKB TR-99-25, 1999a.

10. Svensson, U; A laboratory scale analysis of groundwater flow and salinity distribution in the Äspö area, SKB TR-99-24, 1999b.

11. Svensson, U; A continnum representation of fracture networks. Part I: Method and basic test cases, J. Hydrology, 250, 170-186, 2001a.

12. Svensson, U; A continnum representation of fracture networks. Part II: Application to the Äspö Hard Rock laboratory, J. Hydrology, 250, 187-205, 2001b.

13. Svensson, U; Groundwater flow, pressure and salinity distributions around the prototype repository, SKB report, in prep.

# Sustaining and Applying Regulatory Competence for the Swedish Deep Repository Programme

Neil A Chapman

Radioactive waste regulators have a clear statutory role to rule on applications submitted by the implementor and provide advice to decision-making authorities within government. They have another function that is usually not identified specifically, which is to provide confidence to the public that developments that have an apparent hazard potential are under strict scrutiny and control.

In the former role, the regulatory authority needs to display:

- detailed knowledge of the generic background to proposed developments;
- detailed knowledge of the specific proposals of the implementor;
- complete familiarity with international standards;
- understanding of parallel developments in other countries;
- a scientific and technical capability to evaluate implementor proposals in a timely fashion.

The latter function, in particular, requires that the regulator must also demonstrate:

- independence of the implementor and, to some extent, of government;
- that the standards that it applies are in the best public interest;
- a level of understanding of safety issues at least as good as that of the implementor;
- strength and authority to act and to have its requirements put into practice.

At the same time, few people would expect the regulator to have the same level of detailed knowledge about the implementor's projects as does the implementor itself. Instead, the regulator is expected to have *sufficient knowledge*, combined with the understanding and insight to be able to identify important issues and ask the right questions. This raises the obvious question of *what* knowledge and capabilities the regulator must maintain in order to carry out its job in a thoroughly credible fashion. This is the topic of this short note.

## Where is SKI Now?

SKI has been developing its regulatory capabilities with respect to deep geological disposal of long-lived wastes for more than two decades. So far, owing to the state of development of SKB's programme, it has only been called on to use these capabilities to comment on implementor R&D and siting strategy, and to give advice to government to guide the SKB programme. This situation will soon change, as the SKB programme moves into higher gear, with the anticipated nomination of a preferred site for the SFL facility and consequent applications to proceed with development. At the same time, SKI has had to deploy much of its expertise in geological disposal issues to actual licensing activities for the SFR repository.

Over the last ten years or so, by identifying and sponsoring necessary R&D, and mounting large multidisciplinary projects, SKI has built up capabilities both internally and within a group of contractor companies and individual specialists, in the following broad areas:

- systematic approaches to performance and safety assessment;

- geology and hydrogeology;
- geochemistry and hydrochemistry;
- engineered barrier and waste form degradation;
- environmental change;
- radionuclide transport modelling.

In doing this, SKI has developed its own databases of FEPs and of geochemical information, and its own models and computer codes for structuring PA and for radionuclide transport modelling. Not only has it developed its own, in-house capabilities by testing these resources in projects such as INTRAVAL, Project 90 and SITE-94, but also, importantly, it has built-up a group of experts familiar with the issues that are going to arise in the next few years.

But, times are changing. In many ways, the last decade can be seen as a time of preparation, testing and training for SKI, both internally and externally. SKI must now focus on being ready to apply its capabilities to real licensing of a deep repository facility. Nevertheless, this licensing process is going to extend for more than another decade, during which the SKI capability will need to be kept under constant review and be updated as necessary. Consequently, SKI is faced with the dual responsibility of keeping outward looking and up to date, at the same time that it needs to put the majority of its effort into specific licensing work.

This brings us back to the question of *what* knowledge and capabilities SKI must maintain in order to carry out its job in a thoroughly credible fashion. What activities does SKI need to support in order to have the characteristics identified in the first two groups of bullet points in this note? What is an appropriate strategy that brings together data, consultants, expertise, opinions and PA and other tools, and make best use of them in the run-up to looking (first) at SKB's 2005 interim safety submission?

### Difficult Issues – Making the Best of R&D

There are some difficult issues to be considered when these questions are raised. But SKI needs to look at them now if it is to be in the best position to do its job and to have got there by efficient use of its resources. The first concerns the size and scope of a regulator's basic R&D programme.

It must be accepted that there may be only limited requirement now for SKI to fund more, fundamental R&D. The reason why SKI appears to have looked into some R&D areas in the past is twofold:

- it had identified an issue about which there was insufficient information, either generically or in the specific context to SKB's plans, which it needed to explore to satisfy itself that it was, or was not, important;
- by researching the issue, it has built up an essential expertise in that topic for subsequent regulatory use.

At some point, SKI will have sufficient knowledge to understand the significance and main factors involved in that topic. If the topic is then identified as an issue of potential relevance to SKB's submissions, it is simply SKI's responsibility to request SKB to investigate the matter and report back. Thus, at some point, it is no longer the regulator's responsibility to do more R&D. Earlier, I noted that SKI needs only to understand matters sufficiently well to be able to spot gaps, errors and inconsistencies, and to ask SKB the right questions. Are there some areas that we could identify where this point has been reached? In my view, in the light of the key components of SKB's safety concept being preservation of the EBS in a stable geological environment, it would certainly be worth taking a detached look at whether more work is needed on:

- sorption and solubility databases and models;
- thermodynamic reaction models;
- radionuclide transport models;
- gas generation and movement modelling.

On the other hand, there may be areas that still match the two reasons for doing R&D identified above. SKI might wish to consider whether it knows enough about the_following issues to be able to track and test SKB rigorously:

- seismic impacts on fractures, rock movement and EBS behaviour;
- homogeneity and stability of bentonite resaturation and physicochemical properties;
- copper container degradation and failure modes and times;
- spatial variability of groundwater flow and how it varies with time.

These are issues where, without some developed thinking of its own, it could be hard for SKI to do other than to accept the approaches and conclusions advanced by SKB. At the end of the day, it would not do for SKI to have any residual 'uncomfortable' feelings about these topics.

Closing down on R&D areas will not help SKI to sustain its capabilities, only to make better use of its resources. In parallel, SKI needs to make best use of the expertise that it has built up in its R&D consultants. The best way of integrating and focussing all the diverse facets of that expertise may be more regular review and analysis of the key regions of the disposal system by small teams that work closely together, supported by a programme of limited PA work. These two suggestions are developed below.

### Use the Systems Approach to Organise the Experts!

The first component of the proposed approach is that SKI, using its expert consultants, develop a set of 'state-of-the-art position papers' on key issues that will underpin its tracking of SKB over the next few years. These could be produced by expert elicitation sessions with consultants and highly focussed mini-workshops on specific topics to explore consensus views and areas of continued uncertainty.

These groups would operate as **Clearing Houses** and would supplement the information that SKI has built up in the documentation that supports its Systems Approach, developed during SITE-94 and most recently applied in the last SFR licensing review. The present workshop effectively uses the Clearing House structure, but this would need to be formalised and used regularly, with specific programmes, over the intervening periods. Clearing House memberships and working would need to be established and a programme of work for each agreed. SKI will get better value from its experts if they work together routinely, in a structured manner. Without this approach, the onus of ensuring that there are no gaps in its capability (knowledge, etc) falls entirely inside SKI, as its experts in allied areas meet only infrequently.

The Systems Approach developed by SKI was difficult and time-consuming to build. At times, it felt as though constructing the methodology and system definitions was dominating the practical application. But the hard work has been done now and the graphical structures and supporting documentation bases provide a fine resource that can now be used properly. The PIDs already built would be useful to aid discussion (at whatever level of detail) and the FEP database provides a baseline from which to build to a properly documented SKI 'position paper' on key areas. These areas need to be defined, but could include:

- container degradation;
- bentonite property evolution;
- fracture network flow models;
- data selection, authentication and integration in PA.

Each position paper would act partly as an 'issue resolution' tool with SKB (where SKI can agree to an approach or to a common conceptual understanding) and partly as a challenge to them, to sort out problems.

As the SKB programme focuses-in, the topic of 'issue resolution' will become increasingly important. A clear methodology for handling this (and publishing the results) needs to be in place by the time of the first formal licensing submission. In the run-up, SKI could use its Clearing Houses and the state-of-the-art reports to identify issues that are related largely to concept. Working with SKB to address these issues could then help to develop and test an approach.

### Focus Effort via Limited PA Campaigns

Understanding of the relevance and inter-relationship of issues can only be achieved in an integrated sense using PA. The second component of the suggested approach is thus applying SKI PA expertise in limited but regular 'campaigns' to address issues as they arise. These campaigns could test different models/understandings of key parts of the disposal system in turn, or at appropriate times in the SKB siting programme as field data or interpretations become available.

This programme cannot be as comprehensive as earlier exercises (e.g. SITE-94), nor does it need to be (past exercises were largely used to develop PA capability). SKI has now developed software tools for looking at the disposal system at any level of detail (provided there is an adequate system model) and any level of specificity to site or materials (e.g. SPARTA and AMBER). Over the next two to three years, it should use these to consolidate its own understanding of system behaviour and the relative importance of its components under different circumstances (scenarios), and to help it develop questions for SKB. Later, SKI will need to use these tools to perform an *independent* check on elements of SKB's performance assessment and on its overall safety assessment results.

What might be appropriate points of focus for such a programme? Part of SKI's strategy could be to use PA in limited campaigns to assess the issues that the Clearing Houses are looking at. There is also an obvious link with the Site Characterisation Group (INSITE). Within the next 12 months or so, INSITE is likely to have site-specific questions that some high-level, scoping PA modelling might help with, or which might feed through into the topics the Clearing Houses are looking at.

Topics for the short PA campaigns could be decided and prioritised at annual meetings such as the present workshop, by meetings of Clearing House leaders or by input from the INSITE group.

## Making Regulatory Decisions

A paper from an implementing organisation at the October 2001 ICEM meeting in Belgium was entitled *'Making a Safety Case: More than just Presenting Numbers.'* Similarly, the regulator has to use much wider information than simply a test of compliance with quantitative regulatory targets when reaching a licensing decision. Indeed, ICRP recently emphasised that such compliance, or lack of it, is not alone a basis for accepting or denying an implementor's application. Thus, it would not be enough for SKI's work over the next few years to focus only on the scientific basis for dose and risk estimates.

There are several areas where SKI will need to put the work that has been discussed above in context. For example, it will need to consider how it will:

- address and react to uncertainties and ranges in quantitative SA results;
- want to see scenario likelihood presented;
- weight scenarios that produce elevated doses;
- define the right stage in the SKB programme to resolve the human intrusion issue;
- utilise comparisons with natural radioactivity.

Above all, it will need to think about how it will present its decision-basis to the public, both in a transparent ongoing fashion over the run-up period, and when a license decision is eventually required. Covering these issues may require a separate strategic project on 'regulatory application' in parallel to the more scientific issues discussed so far.

## Moving Forward

In summary, this note proposes that SKI consider the following approach to help sustain and apply its regulatory competence over the next couple of years:

- an early critical review of essential R&D areas;
- organisation of expertise within structured Clearing Houses;
- Clearing Houses tasked to produce state-of-the-art position papers;
- campaigns of PA work to address issues from Clearing Houses and INSITE;
- formulation of a prototype issue resolution procedure;
- starting a small, strategic 'regulatory application' project.

The present workshop is an opportunity for the Working Groups to try to identify 'residual' R&D issues where there is a clear and obvious need for more work, and those where enough has been done. It could also begin to think about the structure and *modus operandi* of the Clearing Houses: their membership, their tasks and objectives for next year.

This note has discussed the regulatory competence issue from an entirely SKI perspective. There are clearly important and overlapping areas that involve SSI, including the biosphere and waste inventory definition. These should not be overlooked.

# Formulation and Presentation of Risk Assessments to Address Risk Targets for Radioactive Waste Disposal

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The recent introduction of a risk criterion in the regulations governing the disposal of radioactive waste in Sweden [SSI FS 1998:1] has prompted SKI and SSI to examine their own assessment capabilities and review methodologies to determine whether changes might be required, or further guidance developed.

The risk criterion states that the annual risk of harmful effects after closure should not exceed $10^{-6}$ for a representative individual in the group exposed to the greatest risk. However, the principal reason for the use of a risk criterion in regulation is not simply to introduce a new or different criterion, but to introduce a means of assessing and evaluating the uncertainties inherent in the description and analysis of the disposal system.

Uncertainty can be classified into two types:

- Epistemic or subjective uncertainty is associated with data from site characterisation and laboratory experiments. In principle, measurements can be made to reduce such uncertainties - although in some cases they may be extremely expensive or even impractical.

- Aleatory or stochastic uncertainties are associated with events for which there is not, and cannot be, observational data. An important example is future human actions, for example the probability of future human intrusion into a disposal system.

Risk assessments are most effective if they account for the first of these uncertainty types probabilistically. Other approaches may be needed to address the second type of uncertainty.

The results of risk assessment calculations should not be regarded as a rigorous statement of system behaviour. Probabilistic risk assessments are intended to help in system understanding, by ensuring that all parts of the potentially complex parameter space generated by combining independent uncertainties are explored.

In contrast to probabilistic risk calculations, deterministic calculations focus on only one part of parameter space. If only deterministic calculations are conducted, then a priori assumptions, supported by best estimates and similar judgements, are required to identify the most important part of parameter space. Deterministic calculations that are conducted in concert with probabilistic risk calculations can be more readily focused.

Adoption of a combined probabilistic/deterministic approach to risk assessment calculations leads to two observations.

- First, although some development of assessment codes will probably be required so as to allow the use of probabilistic inputs and the calculation and display of alternative outputs, there should be little need for changes to conceptual or mathematical models. A possible exception is detailed models with long run times that cannot sensibly be run probabilistically. These may require the development of simplified models calibrated to the more detailed models.

- Second, effort expended in developing probability distributions for risk calculations should be related to the role of the calculations. In other words, defining a large number of probability distributions in terms of simple distributions covering a reasonable range of parameter values is more valuable in terms of building system understanding than costly elicited distributions for a few parameters. There is a role for elicitation in the development of probability distributions, but its use should be focused on key parameters where there are difficulties in establishing distributions. In all cases, traceability and transparency should underpin judgements. Documentation plays a pivotal role in confidence building.

The interpretation of risk assessment results is as important as the conduct of the calculations, and SKI and SSI will need to develop approaches for interpreting the results of their own and the proponent's calculations. Well-established graphical and statistical techniques are available to assist in the processing and understanding of large amounts of data. Beyond the stage of developing a system understanding, however, lies the need for decision-making. A simple comparison of a single risk value (e.g., the mean or expectation value of risk) with a criterion is not enough. There is also a need to examine the distribution of dose leading to the expectation value. Establishing a further criterion, such as the 95th percentile lying below a certain value, may guide a decision but is likely to be too prescriptive for use in all circumstances. In the end, decision-making is a judgemental task and cannot be subsumed to a numbers game.

Notwithstanding these observations with regard to the treatment of epistemic uncertainty, the introduction of a risk criterion to regulations does not help in the assessment of aleatory uncertainties. Assigning probabilities to aleatory uncertainties involves undue speculation and would be arbitrary.

The Swedish regulations require a separate consideration of future human intrusion, which is a principal source of aleatory uncertainty in evaluating the risks associated with radioactive waste disposal. An assessment of aleatory uncertainties through the use of stylised scenarios has also been proposed recently by the International Commission on Radiological Protection (ICRP), and it is clear from these and other regulations and assessments that conduct of a range of standalone consequence or conditional risk assessment calculations is an effective way of exploring uncertainty. However, the interpretation and use of results for decision-making may require the development of additional compliance criteria. The ICRP has proposed the use of doses similar to those that would justify intervention as possible criteria for evaluation of the impacts of future human intrusion.

In the case of aleatory uncertainties, therefore, no developments are considered necessary for the assessment models in use. However, further work and guidance on the treatment of this type of uncertainty, on compliance criteria and on decision-making may be required.

# A regulatory perspective on needed improvements to models of near-field radionuclide transport

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## Introduction

The site investigation phase of Sweden's nuclear waste program is planned to start in 2002 (SKB 2000). Safety assessments conducted periodically and in parallel with the site investigations will play an important role in the decision-making process as to whether a license should be granted for construction of a KBS-3 repository at one of the sites in question (or others). In view of these plans, the present seminar on radionuclide transport modeling comes at an opportune time. The objective of the seminar is to assess the current status of such models, and to set up an agenda for future work targeting specific data, knowledge and tools that must be available to SKI by the time licensing activities begin (2006-2008). Remarks along these lines for models of radionuclide transport in the near field are summarized in the present paper.

Radionuclide transport is taken here to refer to the movement of radionuclides through an environment determined by features, events and processes (FEPs) that control the thermal, hydrologic, mechanical and chemical evolution of the near field. Remarks that follow are heavily skewed in favor of those FEPS that have not, in my opinion, been satisfactorily dealt with in previous safety assessments carried out by SKI and SKB. These older assessments were intended primarily to demonstrate the robustness of the KBS-3 concept. They did not have to provide detailed investigations of all potential issues relating to the performance of the engineered and natural barriers. There were no requirements to use data from a complete site investigation, or to provide the scientific basis underpinning decisions as to whether the repository should be located at a particular site. In contrast, the upcoming assessments will provide essential input to the decision-making process. They must therefore be sufficiently complete that it can be concluded with some confidence on the basis of available knowledge that there are no unaddressed issues that would be so serious as to make it impossible to construct a repository that fulfills long-term safety requirements.

The following remarks are based on review comments from various sources on the recently completed safety assessment, SR 97 (SKB, 1999a), and work completed within the past few years by SKI, SKB and other international programs. Individual components of the EBS (spent fuel, canister, buffer/backfill) are first considered separately. Other comments addressing the thermal, hydrologic, mechanical and chemical evolution of the near field as a whole, and basic data supporting radionuclide transport calculations, are then summarized.

## Spent-fuel issues

A variety of fuel types will be disposed of in a KBS-3 repository (SKB 1999b), including BWR fuel (5,000 tons), PWR fuel (1,500 tons), MOX fuel (23 tons) and 20 tons of spent fuel from the Ågesta reactor. BWR fuel of type SVEA 96 with a burnup of 38 GWd/tU is the reference fuel in SR 97. It consists of cylindrical pellets of sintered ceramic uranium dioxide. The pellets are 11 mm long and have a diameter of 8 mm. The pellets are stacked in Zircaloy cladding tubes, about 4 m in length. A fuel assembly contains 96 cladding tubes, and also contains channel, handle and spacer parts made of the nickel alloys Inconel and Incoloy, as well as stainless steel.

## Inventories

There are potentially significant uncertainties in the total inventories of some radionuclides estimated using ORIGEN-type calculations (Grambow, SKI 2000). Other uncertainties exist in the distribution of nuclides among the spent fuel matrix, the gap between the fuel and cladding, grain boundaries in the matrix, and metal parts of the fuel assembly [the latter three distributions comprising the "instant release fraction" (IRF) in SR 97]. Uncertainties up to 600% are estimated for the total inventories of Se-79 and Sn-126 based on characterization data for spent-fuel testing material ATM 104 (Guenther, 1991). Grambow (SKI 2000) suggests that the uncertainty in the total inventory for Cl-36 used in SR 97 may be as high as 700%, based on the range of total inventories estimated for this nuclide in recent international safety assessments, and that the pessimistic IRF for Cl-36 should be increased from 12% to 15% (i.e., 6% from spent fuel and 9% including metal parts). Associated safety consequences could be significant because Cl-36, as well as Se-79 and Sn-126, are important contributors to dose (SKB 1999a). An effort is needed to reduce these uncertainties to the extent possible, and to account for their effects on total radionuclide inventories and IRFs in future assessments.

## Models of fuel dissolution

Uncertainties remain in fuel dissolution models (SKB, 1999b; Grambow, SKI 2000). The model used in SR 97 accounts for $\alpha$- and $\beta$-radiolysis of water adjacent to fuel surfaces, decomposition and recombination reactions among radiolysis reactants and products, and oxidation-assisted dissolution of $UO_2(c)$. It is assumed that a high partial pressure of $H_2(g)$ can be sustained in the near field by corrosion of the canister's iron insert. It should be emphasized with this in mind that the SR 97 model appears to be inconsistent with results from recent experiments showing that the combination of high $H_2(g)$ overpressures (5 MPa) and a $\gamma$ radiation field strongly suppresses the dissolution rate of spent fuel (King et al., 1999). It is also noted that the approach used in SR 97 to characterize the source term is not quantified based on experimental results accumulated over many years (Forsyth, 1997), but rather on theoretical concepts whose quantification is poorly documented (Grambow, SKI 2000).

The treatment in the SR 97 fuel-dissolution model of reactions involving hydrogen radicals, $H^\bullet$, produced by the radiolytic decomposition of dissolved $H_2(aq)$ is questioned by Grambow (SKI 2000). These radicals are assumed to react with $H_2O_2(aq)$ to form water molecules and $OH^\bullet$. The predicted concentrations of the hydrogen radicals are significantly higher than are calculated using alternative models of water radiolysis, however. This is because a reaction sequence involving: 1) decomposition of $H_2O_2(aq)$ into $O^\bullet$, 2) recombination of $O^\bullet$ to produce $O_2(aq)$, and 3) reaction of $O_2(aq)$ with $H^\bullet$, is not considered in the SR 97 model. The calculated concentration of hydrogen radicals is thus higher than would be calculated using alternative models of water radiolysis, which include this reaction scheme. The elevated concentration of hydrogen radicals reduces the concentration of $H_2O_2(aq)$ available to react with the fuel. Model calculations of fuel dissolution rates ($10^{-8}$/year, SKB 1999b) may therefore be too low. Other sources of uncertainty in the model are attributed to the assumed reaction order for heterogeneous reactions, and the fact that associated rate constants are derived from experiments involving unirradiated $UO_2$(c) rather than spent fuel (SKB 1999b; Grambow, SKI 2000).

The fuel-dissolution rate is also assumed to be time invariant in SR 97. Grambow (SKI 2000) suggests this is reasonable when the radiation field around the fuel is high because radiolysis is then expected to be so dominant that the effects on dissolution rate of time-dependent variations in near-field chemistry (i.e., Eh, pH, $pCO_2$(g), etc.) would be masked. The intensity of the radiation field will decrease with time, however, and the geochemical environment may therefore become more important over the longer term. If so, then mass-transport processes leading to time-dependent variations in near-field chemistry may have to be accounted for in fuel-dissolution models. It is possible, however, that such variations will be minimized by the intrinsic chemical buffering capacity and buffer intensity of engineered barrier materials (Arthur and Zhou, 2000).

More work is needed to reduce the uncertainties noted above. There is in particular a pressing need to develop credible estimates of a "pessimistic" fuel dissolution rate. A pessimistic rate was not established in SR 97 . It can be expected that SKB will continue to improve the fuel dissolution model with a view toward better integration of theoretical concepts with the large body of available and highly relevant experimental results. A parallel effort within SKI is needed to track progress in the modeling work, and to evaluate alternative models and data.

## Canister issues

The canister is designed to fully isolate the waste. SKB's canister design calls for an inner insert of cast iron and an outer shell of copper. The insert provides mechanical strength. The copper shell protects against corrosion. The canister is expected to remain intact for at least 100,000 years, and, if so, this isolation capability alone would be sufficient to ensure safety (SKB 1999a). An alternative scenario, the canister-defect scenario, is considered below.

The canister-defect scenario assumes that a 1 $mm^2$ circular hole (generated by cracking or discharges from the electron beam welder) or a circumferential crack (due to lack of fusion) occurs in the weld between the lid and canister body, and is undetected during inspection for quality control. One canister is assumed to have an initial defect in the realistic case. Five canisters are assumed to have initial defects in the pessimistic case. Both the defect size and total number of defective canisters strongly influence radionuclide releases to the far field (SKB, 1999a). Future refinements to these assumptions will be made as experience is gained in the manufacturing process.

Bond et al. (1997) and Takase et al. (1999) model the hydromechanical evolution of a defective canister. An important result is that $H_2$(g) generated by the anaerobic corrosion of the iron insert would quickly build up a gas counter pressure equal to the hydrostatic pressure, thus limiting the amount of water that could enter the canister from the buffer. These processes in effect give rise to an entirely new safety function. Model results suggest that radionuclide releases from the near field would not occur for 200,000 years because this is the period of time needed to develop a continuous water pathway between spent fuel and the near-field rock.

SKB's hydromechanical models may not adequately capture all relevant processes in the evolution of a defective canister, however. Arthur and Zhou (SKI 2000) suggest that chemical processes are excessively simplified in the models because the real system inside a defective canister is open with respect to the chemical system inside the buffer. Transport of $CO_2$ and $H_2S$ from the buffer could stabilize corrosion products of the iron insert other than magnetite. Corrosion of the insert apparently involves condensation of water vapor to liquid $H_2O$, but it is unclear whether condensation can occur inside a defective canister. Arthur and Zhou speculate that liquid water could form by capillary condensation, but only if pores in the corrosion product layer are smaller than pores between mineral grains in the buffer. The hydromechanical models also appear to neglect leakage of hydrogen through the buffer via dissolution in the buffer's porewater. SKI questions whether certain assumptions used in SKB's models dealing with mechanical effects on the canister are realistic (SKI, 2001). It is assumed, for example, that the copper shell is breached if deformation resulting from growth of corrosion products exceeds 29%. Creep may control canister failure, however, because the corrosion process is very slow and the creep fracture strain is considerably lower than 29%.

In summary, the hydromechanical models apparently neglect a number of processes that are strongly coupled. The evolution of such systems may be highly sensitive to minor variations in initial states, boundary conditions, rate constants and the impact of secondary processes that have not been considered in SKB's analysis. It is concluded that the models do not provide an adequate basis for excluding the possibility of dose exposure before 200,000 years (SKI 2001). SKI recommends that SKB should prepare a more detailed analysis of canister evolution, taking into account rate-determining mechanisms, kinetic data, the evolution of chemical conditions inside the canister, and associated mass-transport processes in the near field. A parallel effort is needed by SKI to evaluate model results, and to consider alternative models and data.

## Buffer/Backfill issues

A buffer composed of bentonite surrounds the canister. The buffer plays a key role in maintaining stable and favorable conditions near the canister surface. The buffer should ensure that: 1) the supply of corrodants to the canister surface is limited by diffusion and reaction with buffer minerals, 2) microbial processes near the canister (e.g., sulfate reduction) are limited, and 3) the migration of radionuclides from an initially defective canister is limited by diffusional transport and sorption onto buffer minerals. The backfill comprises a mixture of crushed rock and bentonite. The function of the backfill is to seal access to deposition tunnels so that rapid transport pathways are not formed, and to limit radionuclide migration by sorption onto backfill minerals.

The chemistry of buffer porewaters will affect the mechanism and rate of spent fuel dissolution, the corrosion behavior of copper and iron components of the canister, and the solubility, speciation and sorption behavior of radionuclides . Attempts to characterize the in-situ chemical composition of buffer porewaters at repository relevant compaction densities have met with limited success because results are complicated by ambiguities arising from the sampling technique used (i.e., centrifugation, compression or displacement - see Muurinen et al., 1996; Muurinen and Lehikoinen, 1997). These complications are due in part to the existence of at least two types of water, which vary in relative proportion depending on compaction density: 1) water that is more-or-less bound to clay surfaces by electrostatic and van der Waals forces, and 2) water that is free from the effects of these forces (Pusch et al., 1990). Geochemical models that account for differences in the properties of bound and free water (e.g., the dielectric constant) are unavailable. Models discussed in the following paragraph assume that all water in the buffer is free water.

The evolution of porewater chemistry is described by SKB using a limited set of ion-exchange reactions involving the smectite clays, and dissolution/precipitation reactions among "impurity phases" (e.g., calcite, pyrite). Other processes, including transformation of smectite (i.e., montmorillonite) to illite and precipitation of minerals and amorphous solids during the thermal period of repository evolution, are also considered by SKB, but these processes are believed to have little potential for adverse impacts on buffer performance. SKB's model of buffer porewater chemistry may, however, be overly simplistic. Alternative models of smectite-water reactions account for additional exchange reactions on tetrahedral and octahedral sites, and are thus consistent with the variability in smectite compositions observed in natural systems (Aagaard and Helgeson, 1983; Giggenbach, 1985). Model parameters are constrained in part by the observed range of these compositional variations, and thus do not rely solely on the results of short-term experiments. In contrast, parameters in SKB's models are constrained entirely by such experiments, and it is therefore unclear whether these models are appropriate for predicting long-term behavior (Arthur and Wang, 2000). SKB's model may also need to be reconsidered in relation to geosphere conditions that could arise in future scenarios of repository evolution. Although illitization may not be an important process in dilute groundwaters, seawater intrusion in a climate change scenario may accelerate this reaction because these solutions contain high concentrations of potassium (Glynn, SKI 2000). The alternative models should be further developed and evaluated in comparison to SKB's model to better gauge the impact of associated conceptual uncertainties on both the short-term and long-term evolution of porewater chemistry. Improvements to existing techniques for sampling porewaters in-situ, or development of new techniques, could provide an experimental basis for development of more realistic models that take into account double-layer effects on the properties of water.

Reviews by Karnland (1998) and Dixon (2000) suggest that salinities as high as 100 g/l will not significantly affect the swelling pressure and associated transport properties of highly compacted bentonite (saturated density ~ 2000 kg/m3). The density of backfill, consisting of crushed rock and bentonite, is much less than that of the buffer, however, and the effect of salinity variations on the swelling pressure is therefore more pronounced. Dixon (2000), for example, concludes that for porewater salinities in the range of 10 to 75 g/l the backfill's effective dry density must be at least 900 kg/m3 to sustain swelling pressures of at least 100 kPa. If swelling pressures in this range are not attainable, then the backfill may not develop a tight seal at the host-rock surface, and rapid transport pathways could thus form. Vieno (2000) proposes several engineering solutions to this potential problem. They involve changes to the type of bentonite used (e.g., Friedland clay vs. MX-80), increasing the proportion of bentonite to crushed rock, and/or changes in repository design. If similar changes are considered necessary to the Swedish KBS-3 design, associated impacts on safety should be assessed.

The effects of emplacement defects in the buffer or backfill have not been evaluated to the level of detail considered in SR 97 for the canister defect scenario. Defects may arise during the acquisition of buffer/backfill materials (e.g., resulting in inhomogeneities in mineralogy), manufacturing of bentonite blocks, emplacement of bentonite blocks, and resaturation. The possible impact of such defects within the framework of repository operations and safety assessment should be assessed.

## Issues related to near-field evolution

The initial state of the repository may include materials that are not normally considered in a safety assessment. These materials include cement plugs at the bottom of deposition holes, construction materials and construction effluents, and a variety of hydrocarbons and other inorganic "stray" materials. A method to control these materials and to produce an inventory of their contents at the time of repository closure is needed. An analysis of the effects of these materials and their alteration products on the longer-term chemical evolution of the near field should also be carried out.

Coupled interactions among thermal, hydrologic, mechanical and chemical processes in the near field during the repository's pre-closure and early post-closure period should also be investigated in greater detail. If resaturation occurs more slowly than expected, for example, then heat from the canister will vaporize porewater in the buffer (Sällfors, SKI 2000; Goblet and de Marsily, SKI 2000). The vapor will migrate away from the canister toward cooler regions of the buffer, where it will condense. Vaporization lowers the degree of saturation and increases the ionic strength of residual liquids. The thermal conductivity of the buffer decreases with decreasing saturation, and the temperature will therefore rise. The elevated temperature will speed up reactions, such as illitization, that could adversely affect the buffer's performance. It is also possible that concentrated solutions resulting from partial evaporation of the buffer's porewater will contact the canister at temperatures near the boiling point of water. These conditions could accelerate corrosion of the canister's copper shell (Hermansson and Eriksson, 1999).

## Issues related to data used in transport models

The quality of a safety assessment depends in part on the reliability of data supporting radionuclide transport calculations. For the near field, these data include radionuclide solubilities and transport parameters [distribution coefficients (Kds), diffusivities and porosities] for the buffer and backfill.

Thermodynamic data supporting estimates of radioelement solubilities are reliable in many cases (e.g., the trivalent and quadravalent actinides), but additional work is needed to improve the reliability of thermodynamic data for some fission products and activation products that can have an appreciable impact on dose (e.g., Se, Sn). Procedures need to be established for the development, management and quality assurance of thermodynamic databases used in safety assessments, which thus include data for both radioactive and non-radioactive elements. Approaches to deal with uncertainties in calculated radionuclide solubilities may need to be refined in future safety assessments (Ekberg, SKI 2000).

Stenhouse (SKI, 2000) points out that Kds are conditional constants that are only strictly valid for a given water composition. Confidence in the use of a set of Kd values therefore depends on the reliability of models of the long-term chemical evolution of porewaters in the buffer and backfill. Stenhouse also notes that Kd values determined using batch experiments are often associated with major errors. Retrieval of Kd values from diffusion experiments is more reliable because these experiments are more representative of expected conditions in the repository.

## Concluding remarks

The main challenge during the upcoming site-investigation phase of Sweden's nuclear waste program, from a regulatory perspective, is the need to attain closure on safety-relevant issues in a timely manner with limited resources. Expert judgment, scoping analyses and numerical models of near-field evolution and radionuclide transport should be used as basic tools supporting the issue-resolution process. These tools can be used to: 1) independently check results put forward by SKB, 2) identify limitations in SKB's models resulting from inadequate documentation, insufficient experimental data or inadequate use of existing data, and 3) evaluate alternative concepts and data. This will help build confidence that there are no unaddressed issues that would be so serious as to make it impossible to construct a repository that fulfills long-term safety requirements.

These tools have of course been used by SKI in past safety assessments. The issue now, however, is whether they are fit for the purpose of licensing activities planned over the next few years. The question at hand is whether existing tools are adequate for this purpose, or whether new or improved tools are needed. It has been noted, for example, that near-field models have historically not been evaluated as thoroughly as models of the far field (SKI 2001). There is clearly a need to correct this imbalance in emphasis, given that all previous safety assessments of the KBS-3 disposal concept have demonstrated that the near field is of primary importance to safety.

It can already be concluded, however, that improvements are probably needed. Some are recommended in the preceding discussion, and others are certain to emerge as a result of this seminar. To these can be added the eventual need to go beyond the current practice of treating individual barriers (fuel, canister, buffer/ backfill, near-field rock) in isolation. To accomplish this, an integrated model incorporating process-level models for each of the barriers should be developed. Although some detail in the process models may be sacrificed to promote computational efficiency, it should be possible to adequately capture essential near-field FEPS by abstracting key results from the process models using expert judgment. An integrated model would permit a more realistic evaluation to be made of near-field conditions arising from time-dependent variations in boundary conditions at the buffer-rock, canister-buffer and fuel-canister interface. The development of a fully integrated model is feasible using modern object-oriented programming techniques, and associated software such as GOLDSIM (http://www.goldsim.com/).

## References:

Aagaard, P. and Helgeson, H. C. 1983. Activity/composition relations among silicates and aqueous solutions: II. Chemical and thermodynamic consequences of ideal mixing of atoms on homological sites in montmorillonites. illites and mixed-layer clays. Clays Clay Miner., 31(3), 207-217.

Arthur, R. C. and Wang, J. 2000. Claystone constraints on models of the long-term chemical evolution of buffer porewaters. In: Scientific Basis for Nuclear Waste Management XXIII, R. Smith and D. Shoesmith (eds.), Mat. Res. Soc. Symp., 608, Pittsburgh, PA, 551-556.

Arthur, R. C. and Zhou, W. 2000. Chemical buffering in natural and engineered barrier systems: Thermodynamic constraints and performance assessment consequences. SKI Report 01:11. Swedish Nuclear Power Inspectorate, Stockholm, Sweden.

Bond, A. E., Hoch, A. R. Jones, Jones, G. D., Tomcyzk, A. J., Wiggin, R. M. and Worraker, W. J. 1997. Assessment of a spent fuel disposal canister. Assessment studies for a copper canister with a cast steel inner component. SKB TR 97-19. Swedish Nuclear Fuel and Waste Management Co., Stockholm, Sweden.

Dixon, D. A. 2000. Porewater salinity and the development of swelling pressure in bentonite-based buffer and backfill materials. POSIVA 2000-04. Posiva Oy, Helsinki, Finland.

Forsyth, R. 1997. The SKB spent fuel corrosion programme: An evaluation of results from the experimental programme performed in the Studsvik Hot Cell Laboratory. SKB TR 97-25. Swedish Nuclear Fuel and Waste Management Co., Stockholm, Sweden.

Geunther. 1991. Characterization of spent fuel approved testing material ATM 104. PNL 5109-104. Battelle, Pacific Northwest Laboratories, Richland, WA.

Giggenbach, W. F. 1985. Construction of thermodynamic stability diagrams involving dioctahedral potassium clay minerals. Chem. Geol., 49, 231-242.

Hermansson, H-P. and Eriksson, S. 1999. Corrosion of the copper canister in the repository environment. SKI Report 99:52. Swedish Nuclear Power Inspectorate, Stockholm, Sweden.

Karnland, O. 1998. Bentonite swelling pressure in strong NaCl solutions – Correlation of model calculations to experimentally determined data. POSIVA 98-01. Posiva Oy, Helskinki, Finland.

King, F., Quinn, M. J and Miller, N. H. 1999. The effect of hydrogen and gamma radiation on the oxidation of UO2 in 0.1 mol dm-3 NaCl solution. SKB TR 99-27. Swedish Nuclear Fuel and Waste Management Co., Stockholm, Sweden.

Muurinen, A., Lehikoinen, J., Melamed, A. and Pitkanen, P. 1996. Chemical interaction of fresh and saline waters with compacted bentonite. VTT Research Notes 1806. Technical Research Centre of Finland, Helsinki, Finland.

Muurinen, A. and Lehikoinen, J. 1997. Model for diffusion and porewater chemistry in compacted bentonite: Experimental arrangements and preliminary results of the porewater chemistry studies. POSIVA 97-02. Posiva Oy, Helsinki, Finland.

Pusch, R., Karnland, O. and Hökmark, H. 1990. GMM – A general microstructural model for qualitative and quantitative studies of smectite clays. SKB TR 90-43. Swedish Nuclear Fuel and Waste Management Co., Stockholm, Sweden.

SKB 1999a. Deep repository for spent nuclear fuel. SR 97 – Post closure safety (vols. I and II). SKB TR 99-06. Swedish Nuclear Fuel and Waste Management Co., Stockholm, Sweden.

SKB 1999b. SR 97: Processes in the repository evolution. SKB TR 99-07. Swedish Nuclear Fuel and Waste Management Co., Stockholm, Sweden.

SKB 2000. Integrated account of method, site selection and programme prior to the site investigation phase. SKB TR 01-03. Swedish Nuclear Fuel and Waste Management Co., Stockholm, Sweden.

SKI 2000. Opinions on SKB's safety assessments SR 97 and SFL 3-5. SKI Report 00:34. Swedish Nuclear Power Inspectorate, Stockholm, Sweden.

SKI 2001. SKI and SSI's joint review of SKB's safety assessment report, SR 97: Review report. SKI Report 01:4. Swedish Nuclear Power Inspectorate, Stockholm, Sweden.

Takase, H., Benbow, S. and Grindrod, P. 1999. Mechanical failure of SKB spent fuel disposal canisters: Mathematical modelling and scoping calculations. SKB TR 99-34. Swedish Nuclear Fuel and Waste Management Co., Stockholm, Sweden.

Vieno, T. 2000. Groundwater salinity at Olkiluoto and its effects on a spent fuel repository. POSIVA 2000-11. Posiva Oy, Helsinki, Finland.

# Experience with the use of General Purpose Modelling Tools in Whole System Performance Assessments

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## 1 Introduction

In September 1998, SKI held a workshop on radionuclide transport modelling. This discussed the way forward for the full range of SKI's modelling capabilities, including research (support) codes and performance assessment (PA) tools. A particular topic of discussion was the need for improved handling of time dependency so that the codes could more faithfully treat time dependency in scenarios.

This paper recaps the issues and ideas from that workshop that are relevant to PA modelling. Our experience in applying a general-purpose modelling tool (AMBER) to the SFR repository as part of the regulatory review of SKB's SAFE project is then set out, demonstrating the power of this approach.

In the light of this, and related, experience we recommend the continued use of such tools for radionuclide transport modelling in PA, and highlight some particular issues that need to be addressed.

## 2 Performance Assessment Modelling Needs

Performance Assessment (PA) modelling is a focal part of a safety assessment. A systematic approach to the analysis of Features, Events and Processes (FEPs), leading to a process model description and a set of scenarios, must ultimately lead to a capability for quantitative calculations. It is generally acknowledged that two distinct types of modelling will be needed in an assessment.

- Detailed modelling (research modelling, support modelling) is used within particular disciplines (e.g. hydrogeology, geochemistry, ecology) to explore the consequences of particular site characteristics, repository design feature, surface characteristics and so on.

- PA modelling (systems modelling) is used to bring together important aspects of all the detailed considerations and expert judgements and to look at the overall system behaviour. In particular, comparisons with regulatory targets are made, although other endpoints will be of interest.

As part of the modelling, it will be necessary to consider the impact of uncertainties in all aspects of the work. The PA modelling will need to have a facility for exploring the consequences of different possible parameter values, and for looking at different conceptual models as well as handling a range of scenarios.

In SITE-94, SKI's main PA tools were CALIBRE (a near-field model for a single spent-fuel canister) and CRYSTAL (a one-dimensional, time-invariant, advection-dispersion model for the geosphere). The biosphere was handled as a steady-state conversion factor, derived from SSI modelling work. A separate probabilistic capability (based on SYVAC) was also available but was not used in SITE-94. The major weakness of the approach used in SITE-94 was the lack of time dependence in the system. It was also difficult to handle “what if” questions that took the conceptual model away from that implemented in the code (e.g. flow in the buffer was not allowed).

When considering the range of different situations in which SKI need to model radionuclide transport, in addition to the range of scenarios to be considered within each assessment, a general-purpose tool is an attractive option. A tool that can incorporate the whole system is also attractive, not least because it removes the need to give special consideration to interfaces between models.

At the time of the 1998 workshop, we had some experience of using AMBER for this type of work (e.g. at the Dounreay site in Scotland). AMBER was originally developed as a compartmental biosphere modelling tool but was being used to model the full system including some complex time dependency (such as cliff erosion). This experience had given us confidence in AMBER’s ability to model a full system.

In the course of the SFR work, some enhancements to AMBER were made to improve its usefulness for this application. The most important enhancements were: Submodel Structure, enabling the system to be visualised in a hierarchical form; Solubility Limitation, allowing non-linear processes to be handled; and Searching, allowing large cases to be checked and updated more quickly.

## 3 PA Modelling in the SFR Review

Four phases of work have been undertaken for the SFR review.

- Demonstration calculations were undertaken in 1999. These calculations demonstrated the capability of the AMBER software to reproduce the key features of the PA modelling undertaken by SKB at the time of the original licensing of SFR.
- Prototype calculations were undertaken later in 1999. These calculations gave confidence in the capability of the AMBER software to meet SKI’s requirements for a PA code and highlighted some important modelling issues for SFR.
- Scoping calculations that were undertaken in 2000; these included consideration of the effects of gas generation and the evolution of the Silo near-field.
- A final set of calculations is currently being undertaken to explore issues arising from a review of SKB’s assessment presented in the SAFE documentation.

A number of time dependent processes have had to be represented including:

- Land uplift, sea level change, and resulting continuous change in the regional Darcy velocity.

- The degradation of engineered barriers, the resulting change in groundwater flows through the near field, and consequential changes to radionuclide transport mechanisms.

- Changing transport velocities in the geosphere resulting in changes to the location and nature of the geosphere-biosphere interface.

Our experience in successfully representing these time dependent processes has provided confidence in the ability of AMBER to represent radionuclide transport at an appropriate level of complexity for PA calculations.

# 4 Conclusions and Recommendations

The experience with SFR shows that the approach of using general-purpose codes can be successfully employed for PA work. AMBER can cope with a wide range of timescales and handles time dependency well. We note that some other general purpose tools are weak in this area.

Areas where there is scope for further improvement include.

- Flow. AMBER does not include a flow modelling capability and so the flow field has to be imposed from outside. The lack of a flow modelling capability means that it is may not be possible to represent groundwater flow in as much detail as desired.

- Copy and Paste. AMBER does not have capabilities for copying part of one case (such as a sub-model) into another. This leads to significant manual effort being necessary in some situations.

- Large systems. Once the system being modelling becomes large, performance is inevitably reduced. There is no reason to believe that AMBER is generally any less efficient than other tools, but nonetheless some improvements would be useful.

- Non-donor transfers. The donor-controlled model in AMBER generally covers radionuclide transport situations well. However this can be a significant limitation in the modelling of, for example, flows of gas.

It is proposed that the approach taken in PA modelling for SFR should be extended to the modelling of SFL.

# The Treatment of Sorption in Performance Assessment

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## 1 Introduction

Sorption, the collective term given to a number of physical and chemical processes governing the uptake of species on solid surfaces, can provide significant retardation for radionuclides, depending on the element concerned. Thus, sorption in the near-field and the geosphere can retard radionuclide transport, thereby allowing significant decay of short-lived nuclides before they reach the biosphere. On the other hand, the sorption of radionuclides in certain reservoirs of the biosphere can increase the potential for prolonged radiological exposure to humans and other species.

Typically for performance assessment (PA) calculations, sorption is represented by the distribution coefficient, or Kd, normally expressed in $m^3\ kg^{-1}$ or $ml\ g^{-1}$. Sorption being an elemental process, sorption databases are generally provided in the form of Kd values for individual elements. Kd values may be determined experimentally, but experimental data are strictly valid only for the conditions under which measurements were carried out. In this context, although having a thermodynamic basis, the Kd approach is an empirical one, and for this reason has been subject to substantial criticism. Thus, any Kd values recommended are representative of a specific set of chemical conditions covering the solid (rock/mineral) and aqueous phases.

Given this brief background, this extended abstract provides a summary of the current status of the treatment of sorption and Kd values in PA as well as some initial reflections on future needs in this area, in advance of the Workshop. The focus here is primarily on the near-field.

## 2 Current Status

The discussion in this section is confined to three topics, viz.

- treatment of time dependency;
- uncertainties in sorption databases;
- mechanistic modelling of sorption.

### 2.1 Treatment of time dependency

The treatment of time dependency in connection with sorption, i.e. how Kd values for certain environments might change with time, has been relatively limited to date. Given the extended timescales associated with PA and safety assessments, however, conditions in the near field and to some extent the far field, cannot be expected to remain close to those existing at post-closure.

This is particularly true in the case of a cementitious near field where cement/concrete phases will change (degrade) significantly over time. Thus Bradbury and Sarott [1995] were first to recommend Kd values for elements based on different states of degradation of cement in a L/ILW repository, and others have followed their lead [Krupka and Serne, 1998); Savage et al., 2000].

In the near field of a KBS-3 repository, the key changes with time affecting radionuclide sorption will include the (slow) formation of canister corrosion products together with the evolving chemical properties of the bentonite buffer under normal or perturbed conditions. Although the expected evolution of bentonite porewaters was evaluated by Bruno et al. [1999], no explicit account was taken of such changes in terms of time-dependent sorption data.

In the far field, the significance in terms of sorption of surface mineral coatings on crystalline rocks, particularly fractures, has been recognised for a long time [e.g., McKinley and Hadermann, 1985]. However, although the sorption of radioelements is expected to occur mainly on such coatings, which exhibit relatively high Kd values, the tendency has been not to take credit for such strong sorption in PA calculations, but rather to incorporate a range of more conservative Kds, thereby allowing for the possibility of future alteration/removal of these surface coatings as the chemical environment changes. Such an approach is reasonable and conservative in the absence of information/data on the longevity of these coatings.

### 2.2 Treatment of Uncertainty

As stated in the introduction, the Kd approach is an empirical one, the value of this parameter will change according to the chemical conditions governing the rock-water or mineral-water systems.

Typically, for deterministic PA calculations, two Kd values are provided as input data. The first value is regarded as a 'realistic', or 'best estimate' of the extent of sorption of a radioelement under expected repository conditions. The second value is intended to be more conservative but its exact nature is arguably more tenuous, being described in qualitative terms such as 'representative of perturbed conditions', 'exploratory', 'pessimistic', or 'less likely'. Frequently, this second value is an order of magnitude less than the first Kd value.

For probabilistic safety assessment calculations, some type of probability density function (PDFs) is assigned to Kd parameter values, as was done for PA work associated within the U.K. Nirex's repository programme [Hooper, 1997], for example. However, the underlying basis for such a treatment is still tenuous, however, also relying heavily on expert judgement, since experimental data rarely exist to support such PDFs.

Whatever the specific approach adopted in PA calculations, there are a number of uncertainties associated with the provision of Kd values:

- Lack of experimental data for certain elements. Clearly, gaps exist in the literature covering the sorption of some radioelements. This situation may be due to practical experimental difficulties, e.g. the inability to distinguish precipitation from sorption, but also may reflect the low degree of importance attached to the sorption of some radioelements, i.e. some nuclides (radioelements) may be a negligible component of the radionuclide inventory, or may not represent a significant radiological hazard. It is not unreasonable to expect that funding be directed towards key (safety-relevant) radionuclides. The use of 'good' chemical analogues can reduce some of the uncertainty in this area.

- Uncertainty in predicting the specific solid surfaces on which sorption occurs, or in predicting the nature of the solid and aqueous phases as a function of time. The latter problem links to the impact of time dependency on sorption discussed above and would include prediction of the evolution of the redox environment, Eh being an important parameter influencing speciation and the extent of sorption of redox-sensitive radioelements.

- Interpretation/relevance of laboratory data, with respect to field conditions. Such problems include taking account of possible increased temperatures for environments surrounding certain types of waste (few sorption data exist for elevated temperatures). More significant difficulties have arisen in extrapolating batch sorption Kd data obtained for laboratory bentonite/water systems (low solid/liquid ratios) to the incorporation of Kd values in apparent distribution coefficients for compacted bentonite systems (high solid/liquid ratios).

- Influence of organic materials degradation products on radionuclide sorption For certain types of repository, particularly a L/ILW repository, organic materials constitute a non-negligible component of the waste inventory. For other planned repositories with no organic wastes, organic materials may be present as additives to concrete. Under these circumstances, the overall impact of such organic materials and, more importantly, their degradation products, on the sorption of radiolements has yet to be defined precisely, e.g. the impact of iso-saccharinic acid (ISA), identified as a product of cellulose degradation, on the sorption of certain actinides.

Awareness of such uncertainties exists, of course, in the course of performing PA calculations. For example, in an effort to address (and accommodate) uncertainties regarding sorption in a quantitative manner, Andersson [1999] provides a series of reasoned arguments in his report covering the compilation of data as input for SR97.

## 2.3 Mechanistic Sorption Models

A more rigorous approach to sorption lies in the application of mechanistic sorption models which provide a thermodynamic treatment of the electrical properties of the mineral surface/water interface. Of these, a class of models, termed surface complexation models (SCMs), have been used successfully to model pH-dependent sorption (for example, Dzombak and Morel [1990]). Such models have made substantial advances over the past decade, not only in increasing our understanding of sorption mechanisms, but also in obtaining necessary input data to support the models. There have been a number of successes in this area, as discussed by Langmuir [1997]: also Arthur [1996], in successfully extending an analytical model of sorption of neptunium(V) on hydrous ferric oxide to the calculation of a whole-rock Kd value using the concept of a surface film; and Heath et al., [1996], in modelling the sorption of caesium and iodide on cementitious phases. Thus, surface complexation models are now routinely incorporated in geochemical codes such as MINTEQA2 [Allison et al., 1991], HARPHRQ [Haworth et al., 1994] and PHREEQC [Parkhurst, 1995].

Some drawbacks still exist in this area, however, for example:

- the fact that modelling is carried out on relatively simple systems, such as single mineral adsorbents, whereas natural systems comprise complex mixtures of a variety of minerals with resultant numerous complexes in the aqueous phase.

- the need for some form of curve fitting of experimental data in order to generate specific constants used in model calculations.

Thus, despite the advances in this area, it is likely that sorption databases of Kd values will still be required for input to PA calculations over the next decade or so. The best use of mechanistic sorption models, therefore, will continue to be to provide support to decisions made on the selection of specific Kd values, particularly for safety-relevant elements.

## 3 Future Needs

Some initial thoughts in this area are provided below.

- *Kd values for compacted bentonite*: Systematic examination and resolution of the differences between certain batch sorption data for bentonite/water systems and corresponding apparent diffusion coefficients (incorporating sorption) for different radioelements. This issue has been addressed in the past, but not explained conclusively.

- *Cementitious systems* will feature to some extent in most types of radioactive waste repositories, certainly in the SFR and planned SFL 3-5 repositories. Thus, sorption of a wide range of radioelements on cementitious phases will be a significant mechanism for retardation in the near field. It is clear, however, that essentially all the sorption data obtained experimentally for cementitious systems involve fresh hardened cement paste as solid phase and, therefore, are relevant to the initial stage of cement evolution. With respect to the three stages of cement evolution ('Environments') identified by Bradbury and Sarott (1995), there are no experimental data relevant to Environment III, the last stage identified in the evolution/degradation of cement, when CSH phases are dissolving, the Ca:Si ratio is decreasing, and the pH is also decreasing. Some experimental work in this area is therefore justified, again focussing on key (safety-relevant) radioelements.

- *Surface complexation modelling*: Some progress has still to be made to achieve a consensus in the use of sorption modelling as a means of supporting the selection of Kd values [NEA, 1997]. In particular, the following issues appear to be key ones to resolve:
  - treatment of mixtures of minerals and consistency in the 'bottom-up' approach when dealing with a mixture of minerals. At the NEA Sorption Workshop in Oxford [NEA, 1997], cases were cited in which a combination of minerals resulted in a smaller overall Kd; in other cases, there was an enhancement in Kd value. However, such reductions or enhancements were not predicted but, rather, were explained in retrospect. Differences such as these must be explained.
  - justification for whether to include an electrostatic term in surface complexation modelling, in an effort to simplify calculations. Given the widespread criticism that the Kd values in sorption databases are not based on rigorous thermodynamic theory, it is important that the contribution for sorption modelling is not exposed to the same criticism.

- *Role of corrosion products*: The potential exists to take some credit for sorption on corrosion products, particularly iron corrosion products which are strong sorbers. An initial attempt was made in this area [Savage et al., 2000], but experimental data are generally lacking, including detailed knowledge of the surface properties of the solid phases expected. In order to take advantage of retardation from sorption on corrosion products which will be a significant near-field component of a L/ILW repository, some experimental work, complemented by modelling, is recommended, focussing on key (safety-relevant) radioelements.

Generally, the overall objective is to reduce at least some of the uncertainties discussed above, although not all uncertainties need to, or can be reduced. Currently, some uncertainties are addressed by providing bounding Kd values to cover extremes in sorption behaviour;. If truly pessimistic (robust) arguments and assumptions are carried into PA calculations and lead to doses well below regulatory limits, then low priority should be attached to carrying out additional work in corresponding research areas.

With or without modelling, the provision of Kd values should be based at least on a solid chemical foundation. On the other hand, although the Kd approach is an empirical one, the situation should not be viewed as pessimistically as it might appear. As noted by Allard [1991] and Bradbury and Baeyens [1993], despite the complexities and heterogeneities of the chemical environments in nature, in most cases only a few processes and subsystems have a key influence on sorption.

## References

Allard, B. (1991); Can distribution coefficients be used for the modelling of radionuclide transport? In: Radionuclide Sorption from the Safety Evaluation Perspective, Proc. NEA Workshop, Interlaken, Switzerland, October 1991. NEA/OECD, Paris, France.

Allison, J., Brown, D. and Turner, D. (1991) U.S. Environmental Protection Agency Report EPA/6003/3-91/021, Washington DC, USA.

Andersson, J. (1999): SR97: Data and data uncertainties. SKB Technical Report TR-99-09. Swedish Nuclear Fuel and Waste Management Company, Stockholm, Sweden.

Arthur, R. (1996): Adaptation of mechanistic sorption models for performance assessment calculations. SKI Report 96:34.

Bradbury M.H. and Sarott F-A. (1995) Sorption databases for the cementitious near-field of a L/ILW repository for performance assessment. PSI Report 95-06. Paul Scherrer Institut, Villigen, Switzerland.

Bradbury, M.H. and Baeyens, B. (1993): A general application of surface complexation to modeling radionuclide sorption in natural systems. Journal of Colloid and Interface Science, 158, 364-371.

Bruno, J., Arcos, D. and Duro, L. (1999): Processes and features affecting the near-field hydrochemistry, groundwater-bentoniter interaction. SKB Technical Report TR-99-XX. Swedish Nuclear Fuel and Waste Management Company, Stockholm, Sweden.

Dzombak, D. and Morel, F. (1990) Surface Complexation Modelling: Hydrous Ferric Oxide. Wiley Interscience, New York, USA.

Haworth, A. and Smith, A.C. (1994) Improvements to the coupled chemical equilibria and transport code CHEQMATE. U.K. Nirex Safety Studies Report NSS/R324. U.K. Nirex Ltd., Harwell, U.K.

Hooper, A. (1997): Sorption in performance assessment – the Nirex perspective. Contribution 1.1, NEA Sorption Workshop, Oxford, May 1997.

Krupka, K.M. and Serne, R.J. (1998) Effects on radionuclide concentrations by cement/groundwater interactions in support of performance assessment of low-level radioactive waste disposal facilities. U.S. Nuclear Regulatory Commission Document NUREG/CR-6377. USNRC, Washington D.C.

Langmuir D. (1997) The use of laboratory adsorption data and models to predict radionuclide releases from a geological repository: a brief history. Mat. Res. Soc. Symp. Proc. 465, 769-780.

McKinley, I.G. and Hadermann, J. (1985): Sorption database for Swiss safety assessment. Nagra Technical Report NTB 84-40. Nagra, Wettingen, Switzerland.

NEA (1997): International Workshop on chemical modelling of sorption in the field of radioactive waste management. Meeting held at Oxford, England, May 6-8, 1997.

Parkhurst, D.L. (1995) Users Guide to PHREEQC – a computer program for speciation reaction-path, advective-transport, and inverse geochemical calculations. U.S. Geol. Survey Water Resources Inv. Report 95-4227.

Savage, D., Stenhouse, M.J. and Benbow, S. (2000): Evolution of the physico-chemical characteristics of the SFR repository. SKI Report 00:49.

# Geochemical Modeling as a tool for Conservative Performance Assessment

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In the assessment of performance of a repository for nuclear wastes, long time properties of barriers, natural as well as engineered play key roles. The work of the modelling group at Dept. of Nuclear Chemistry, Chalmers, has been focused on the chemical properties of these barriers. Although important, mechanical properties as well as inert transport have been outside our areas of study.

## Groundwater chemistry

The chemical properties of future groundwaters in the repository area belong to the most important features of interest in connection with PA. Models have been developed for simulating response of the groundwater to different scenarios and to handle different kinds of unknown properties of the rock - groundwater system. In particular the spatial variability is taken into account. The main program in the suite is the CRACKER program, that simulates groundwater flowing through a flat fracture with minerals randomly distributed across the surfaces. The CRACKER program in combination with a model involving mixing of different ancient waters has been shown to give reasonably accurate descriptions of the groundwaters found currently at ÄSPÖ.

It has been found likely that neither pH nor the redox potential is controlled any simple reaction, e.g. dissolution/precipitation of a certain mineral. Rather, pH and redox potential are likely to be controlled by several different redox reactions, in which minerals as well as redox couples in the groundwater take active parts. The grain size of minerals does not influence groundwater chemistry significantly, but it has a major influence on the possibilities for radionuclides to be retarded by sorption at the fracture walls.

Future works in the area will mainly consist of application to possible future properties of the groundwater at proposed locations for repositories. Some model development is also needed, particularly to include surface irregularities and larger sizes of the fracture systems modelled.

## Radionuclide solubility

Solubility values serve as upper limits for the concentrations in groundwater of radionuclides leaching from the repository in the case of a failure. As will be seen below, the solubilities differ for the cases of dissolution and precipitation. The solubilities at dissolution are upper limits for concentrations of radionuclides leaving the waste form, while solubilities at precipitation are upper limits for the concentrations after contaminated groundwater has undergone some kind of chemical change which causes a decrease in solubility for one or more element.

The purpose of this work has been to determine solubility for some radionuclides in a granitic groundwater at different pH values and redox potentials. At first sight, this appears to be a straightforward task, which has been performed by several authors for different kinds of groundwaters.

The weaknesses with most kind of approaches are that the influence of the dissolution precipitation processes on pH and pE of the aqueous solution. Furthermore, no interactions with the surrounding rock minerals are taken into account. This means that they do not simulate the system which is of concern for safety assessments. As far as the solubilities are low enough, this does not matter, but at increasing concentrations, the influence of the studied element upon the aqueous system cannot be neglected. This happens when the concentration is greater than $10^{-8}$ M and in the case of low redox buffering capacity, at even lower concentrations.

When it comes to solubilities to be used in connection with safety assessments, one has to realise that the solubility of an element is no longer a uniquely defined quantity. Rather, it depends on the circumstances. Thus, dissolution of a solid phase in most cases gives a concentration which differs from the one reached if the same solid phase is precipitated from a solution, which for some reason is supersaturated. One also arrives at different solubility values if the initial or the final pH value of the groundwater is considered.

As solubilities give upper limits for concentrations of radionuclides, the same kinds of calculations have to be performed for proposed repositories.

## Cement degradation

A simplified model for cement has been developed. In this model, the main components of cement are two solid solutions (solid mixtures). One of the solids is almost pure portlandite ($Ca(OH)_2$) while the other is a gel with a considerable content of Si as well as Ca.

Other components are supposed to be a pore water with high concentrations of Na0H and KOH, causing pH values of 13 or more. After a certain period of time, most of the initial pore water has either leached away, or has reacted with carbonates, which tends to lower the pH value to a bit over 12. Aluminium and sulphate phases are also assumed to be present in the cement.

For validation of the model, results from an experimental study of cement leaching with low-saline granitic groundwater have been used. It has been found that the experiments and the simulations agree fairly well concerning the concentrations of the major components of the leachates.

## Sorption of radionuclides in cement

In addition to being a physical barrier, cement also is able to sorb considerable quantities of many radionuclides. In the sorption model, cement is assumed to consist of the gel phase and a phase that is almost pure portlandite, $Ca(OH)_2$. Both can be considered as solid solutions, which means that they are able to incorporate different elements into their structure. Of these two phases, portlandite is rather compact while the gel phase has a very irregular structure, probably fractal. This suggests that sorption essentially takes place as absorption in the gel phase. A model has been developed for handling sorption in this way. Essentially, Kd remains constant as far as the concentration of the radionuclide is reasonably low, but it will depend on pH of the surrounding solution, and also on the state of degradation for the cement. Essentially, determination of one Kd value is enough to model the development of Kd during the entire degradation process.

The most essential future work is comparison of the model with experiments. If successful, it will be important in modelling of releases from repositories containing cement.

## Uncertainties

Most chemical properties are more or less uncertain. This influences all the areas mentioned above. To handle this, several programs have been developed. The concept of uncertainties and there implications for performance assessments also has been studied.

Uncertainties in the data during laboratory experiments aimed at measurements of thermodynamic constants may cause the amount of some species to have uncertainties of several tenth of the relative mass fraction.

The thermodynamical data obtained in the laboratory may then be used for solubility calculations under different conditions and water compositions. Clearly there are several uncertainties associated with solubility calculations in the rock-water system. First there is the effect of uncertainties in thermodynamic data such as stability and solubility constants, and also enthalpies of reaction if the water is not at room temperature. Furthermore, there are the rock-water interactions which will change the water composition as different minerals come in contact with the water flowing through a system of fractures. Studies in mineralogy to an accuracy good enough for modelling of water evolution are difficult to perform, and therefore the mineral composition of the rock and thus the water composition should be treated as parameters subjected to uncertainties.

In addition to these uncertainties in input data there are also conceptual uncertainties. The calculation of solubility should be an easy task for every chemist, but in fact results differing by orders of magnitude are found even when the modellers have used the same computer program and the same data.

In the future, uncertainties should not be treated separately, but should be included in every model handling the behaviour of a repository.

## Brownian simulation of matrix diffusion

The commonly used approach in dealing with matrix diffusion is to assign an effective diffusion constant for the radionuclide in the rock matrix. The idea behind this approach is

that, on a scale much larger than the pore size, the irregularities tends to cancel out. Although it might look plausible at first sight, this approach has been questioned both for theoretical and experimental reasons.

In our simulations, the Brownian method has been used to investigate the transport of dissolved material in a rock matrix modelled as a system of pores with a wide variability in size and shape. The Boltzmann distribution is used locally, although the system globally is far from equilibrium.

The simulation consists of two main parts. First, the model rock is formed by precipitation of irregular mineral grains from a liquid phase. As the grains grow, they tend to form a mostly solid piece of rock.

In the second part of the simulation, a dissolved species is introduced at one side of the rock and allowed to diffuse through its pore system. It is found that no apparent diffusion constant, D, can explain the properties of the system. Rather, D is found to be a function of both distance and time.

The role of reversible and irreversible sorption remains to be studied with Brownian techniques before it can be applied to real repository conditions. As has been mentioned above, the technique is needed as bulk methods fail to handle the situation.

# Coupled surface complexation and transport of uranium in the Near-field of a spent nuclear fuel repository

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Sorption is a very important mechanism for the retardation of radionuclides in the near field of a repository of spent nuclear fuel. In the performance assessment of the spent fuel, sorption is often modelled as linear equilibrium sorption and described in the mass transport equation by a constant partition factor, $K_d$, between the sorbing phase and the aqueous phase. This factor is then lumped into diffusion coefficient in the mass transport equation. Many field and experimental evidences indicate that this $K_d$-approach has some limitation. The partition factor $K_d$ is a constant only when the water composition is constant for a given sorbing material. When the water composition changes, e.g., with variation of pH, Eh and aqueous phase speciation, the value of $K_d$ changes.

Sorption on the interface of a metal oxide/clay mineral and an aqueous solution has often been treated by surface complexation model. This model has produced successful quantitative descriptions of both cation and anion sorption phenomena, principally because of its use of a combination of concepts taken from coordination chemistry and the theory of the electrical double layer. In addition to sorption on mineral surfaces in the engineered barrier, some radionuclides released from a repository can be reduced by reducing minerals in the near field and re-precipitate.

We use a fully coupled transport/reaction model for the near field of a repository. Sorption of the uranyl species on clay minerals in the bentonite has been quantified by using a surface complexation model. Reduction of the uranyl species by pyrite and precipitation of uraninite and ferrihydrite has also been included in the model. Special attention has been paid to compare the relative importance of retardation of uranyl species by sorption and by reduction/precipitation. With a time-scaling technique, we can extend the modelling time to over millions of years.

Any diffusive transport model using explicit method for solving the system of parabolic equations has limitation in the length of its time step. We have previously developed a time-scaling technique to circumvent this problem. This technique works well with mineral dissolution and precipitation. When sorption by surface complexation is included, caution should be taken to use this technique because it does not scale the proton concentration proportionally and proton is a competing species for sorption. The technique can be used so long as the sorption reactions makes up only a small part of the uranyl dissipation. Then the conditions prevail that allow us to use the pseudo-steady-state approximation that the time scaling technique needs.

The modelling results show that chemical reaction fronts for the dissolution of pyrite and precipitation of ferrihydrite and uraninite propagate within the bentonite buffer. The rate of the propagation depends on the assumption of the concentration of the uranyl species in the spent fuel canister.It is assumed to be $10^{-6}$ M. This value is somewhat arbitrary. When the solubility of uranium is limited by schoepite, the uranyl concentration could be as high as

$3*10^{-3}$ M. However, there is still great uncertainty concerning the redox conditions inside the canister. The water radiolysis may cause it to become rather oxidising, but reduction by high-pressure hydrogen catalysed by the fuel surface may well keep the conditions to be reducing. The uranyl concentration depends directly on the redox conditions in the canister. When the concentration is higher, the rate of the dissolution/precipitation front movement will be higher, and vice versa.

The propagation rate of the redox front also depends on the ferrous iron concentration in the pore water in the granitic bedrock. If that concentration is sufficiently high, it can diffuse through the bentonite and react with part of the uranyl species released from the spent fuel. In this case less pyrite will be oxidised and the redox front will propagate at a lower rate.

The results also indicate that there is essentially no difference between the pyrite oxidation rate when the sorption is included or not. The sorption process competes with the reduction process to retard further transport of the uranyl species out of the bentonite. This result implies that the dominating process for the retention of the uranyl species, possibly also other radionuclides, is the reduction by reducing minerals and subsequent precipitation. The modelling results show that amount of uranium that resides in the uraninite precipitate is 5 to 6 orders of magnitude higher than that in the sorbed phase.

From this study, it can be concluded that:

(1) The uranyl species released from the canister will be sorbed on mineral surfaces in the bentonite buffer only in the region where the pyrite has been oxidised,
(2) The sorption of uranyl species is not an important retention mechanism compared with the process of reduction and precipitation.

In the above modelling approach we have considered only the surface complexation sorption capacity of the clay minerals. Clay minerals like montmorillonite have also a large, mostly cation, ion-exchange capacity, due to the structural negative charges caused by isomorphic substitution of Si by Al. Sorption by the ion-exchange mechanism need to be studied.

In our previous approach, the pyrite will be oxidised and precipitate as ferrihydrite, but the sorption capacity of the newly-precipitating ferrihydrite has not been accounted for. In our future studies, this should be considered.

We have so far only considered the sorption and reduction of the uranyl species. Sorption and chemical reactions coupled with transport of other uranium species and the species of other radionuclides need to be studied.

In the Climate Scenario in SKB's SR-97 report, oxygen-rich glacial meltwater can in the worst case possibly penetrate through the bedrock into the near field of a repository. The reducing capacity may be dissipated and sorption will probably be the only mechanism that can retard the released radionuclides. This scenario need to be studied further.

# Modelling of Radionuclide Transport by Groundwater in Fractured Bedrock for Performance Assessment Purposes

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## 1. Introduction

Transport of solutes in fractured rock is affected by advection in conducting fractures and matrix diffusion as well as sorption onto the solid matrix. Various models have been developed to describe solute transport in fractures subject to matrix diffusion and sorption (e.g. Neretnieks 1980, Grisak and Pickens, 1980 and Wels et al. 1994). Most models do not include the effect of heterogeneity in rock properties and sorption kinetics on solute mass transfer. However, the impact of aperture heterogeneity in an individual fracture on solute transport has been described numerically using particle-tracking simulations (e.g. Moreno et al., 1988). Cvetkovic et al. (1999) analysed the effect of heterogeneous aperture and matrix diffusion on solute transport in a single fracture in terms of two spatially random parameters using a Monte Carlo technique. Recently, Painter and Cvetkovic (2001) extended their analysis of heterogeneous aperture and matrix diffusion to solute transport on a fracture network scale but without account taken to the effect of aperture heterogeneity on the flow distribution.

The purpose of this study is to develop a performance assessment (PA) model for analyses of radionuclide transport in geosphere, in which the model takes into account both the effect of rock properties on mass transfer and aperture heterogeneity on the flow distribution. By using a travel time description of radionuclide transport in rock fractures, we decompose the transport problem into a one-dimensional mass transfer problem and a two-dimensional flow problem. The proposed approach includes numerical simulations of the fluid flow in a discrete feature network and a one-dimensional analytical solution of mass transfer through the series of fractures. The mass transfer model in fractured rock depends on the well-known mechanisms such as advection, dispersion, matrix diffusion and sorption as well as sorption kinetics. Moreover, uncertainty in our knowledge of the heterogeneous rock properties in a fracture network scale can be taken into account. Finally, we demonstrate the use of the proposed PA sub-model and compare the result with that of the one-dimensional transport model similar to the one used in SITE-94 (SKI, 1996) with a case that a pulse of radionuclides releases from a canister and migrates to the biosphere based on data from Äspö site.

## 2. Modelling solute transport in heterogeneous bedrock

To solve the above mentioned transport problem the three-dimensional analysis of the mass flow can be performed by studying the change of the solute mass in water parcels travelling along a large number of trajectory paths. In a Lagrangian framework or a travel time description the transport problem is decomposed into a two-dimensional problem, in which the trajectory paths of inert water parcels are determined, and a one-dimensional problem in which the mass-transfer between the parcels and rock matrix is determined. Here, we can obtain the expected probability density function (PDF) of the residence time for water in the whole distribution of trajectories in the fracture network (Dagan, 1989; Rodriguez-Iturbe and Rinaldo, 1997)

$$< f(t,\tau) >= \int_0^\infty f(t,\tau) g(\tau) d\tau \tag{1}$$

in which $g(\tau)$ is the travel time PDF for a large number of inert water parcels arriving at certain control section for the whole distribution of trajectories in fracture network, $\tau$ is the residence time of an inert water parcel travelling along one of the trajectory paths, and $f(t, \tau)$ is the residence time PDF of solute mass in the water parcel, where $f(t,\tau) = c(t,\tau)/M_0$, $M_0$ is the total mass of the solute inserted into the fracture [kg], c is the concentration of solute per unit volume of water [kg/ $m^3$] and t is the time [s]. In the following sections we describe how $f(t, \tau)$ and $g(\tau)$ can be obtained.

### 2.1 Theory for one-dimensional transport

Transport of radionuclides in fractured rock is affected by advection and diffusion in conducting fractures as well as diffusion into micro-fissures of the rock matrix (matrix diffusion) and sorption onto the solid matrix.

If radioactive decay and surface diffusion are disregarded, a kinematic formulation for the solute mass transport in one dimension can be given as (Xu and Wörman, 1999)

$$\frac{\partial \tilde{c}}{\partial t} + \tilde{u}\frac{\partial \tilde{c}}{\partial x} - E\frac{\partial^2 \tilde{c}}{\partial x^2} - 2\frac{\tilde{e}_t \tilde{D}_p}{\tilde{h}}\frac{\partial \tilde{c}_m}{\partial z}\bigg|_{z=0} = 0 \tag{2}$$

$$\frac{\partial \tilde{c}_m}{\partial t} - \frac{\tilde{\varepsilon}_t}{\varepsilon}\tilde{D}_p\frac{\partial^2 \tilde{c}_m}{\partial z^2} + \tilde{k}_r\left(\tilde{K}_D\tilde{c}_m - \frac{\rho}{\tilde{\varepsilon}}\tilde{c}_w\right) = 0 \tag{3}$$

$$\frac{\partial \tilde{c}_w}{\partial t} - \tilde{k}_r\left(\frac{\tilde{\varepsilon}}{\rho}\tilde{K}_D\tilde{c}_m - \tilde{c}_w\right) = 0 \tag{4}$$

in which $c_m$ is the dissolved solute mass per unit volume of pore water in the rock matrix [kg/ $m^3$], $c_w$ is the sorbed solute mass per unit solid mass [kg/kg], D is the molecular (ionic) diffusion coefficient [$m^2$/s], u is the advection velocity of the solute [m/s], x is a length co-ordinate, h is the fracture aperture [m], E is the hydraulic dispersion coefficient [$m^2$/s], the pore diffusivity $D_p = D\delta_D/\tau^2$ [$m^2$/s], $\varepsilon$ is the total porosity of rock matrix, $\varepsilon_t$ is the porosity of rock matrix available to matrix diffusion, $\delta_D$ is the constrictivity, $\tau$ is the tortuosity, $\rho$ is the density of the rock [kg/ $m^3$], the distribution coefficient $K_D = (\rho/\varepsilon)(c_w/c_m)$ and $k_r$ is the sorption rate coefficient [$s^{-1}$]. Variables marked with a 'tilde' (~) can be assigned as spatially random in the transport direction (x-direction), if the effect of heterogeneous rock properties are taken into account.

The boundary and initial conditions of a solute pulse travelling in the fracture network are defined as

$$\tilde{c}(x=0,t)=\delta(t)\frac{M_0}{Q} \tag{5}$$

$$\tilde{c}_m(L=0,t)=\tilde{c}(x,t) \tag{6}$$

$$\frac{\partial \tilde{c}_m}{\partial z}\Big|_{z=Z}=0 \tag{7}$$

$$\tilde{c}(x,t=0)=\tilde{c}_m(x,t=0)=0 \tag{8}$$

in which Q is the water flow [$m^3/s$], δ(t) is the Dirac delta function [$s^{-1}$] and L is the maximum diffusion depth [m].

Due to lack of space we neglect the analyses of the effect of uncertainties of rock properties on radionuclide transport at this stage (details can be fond in Xu et. al., 2001 and Wörman et. al., 2001). The solution of (2) to (4) with the boundary and initial conditions from (5) to (8) in Laplace domain is

$$\bar{c}=\frac{M_0}{Q}\exp\left[\frac{ux}{2E}-\frac{ux}{2E}\sqrt{1+\frac{4E}{u^2}\left(\frac{p}{E}-\frac{2D_e}{h}\alpha\left(1-\frac{2}{1+\exp(-2\alpha L)}\right)\right)}\right] \tag{9}$$

in which p is the Laplace transform variable and

$$\alpha=\sqrt{\frac{p\left(1+\dfrac{1}{p+k_r}\right)}{\varepsilon_t/\varepsilon D_p}} \tag{9}$$

If we neglect the hydaulic dispersion, i.e., the third term in (2) is neglected, the solution to this problem is as the following and will be used in the travel time approach:

$$c=\frac{M_0}{Q}\exp\left[-\frac{p}{u}x+\frac{2\varepsilon_t D_p}{hu}\alpha\left(1-\frac{2}{1+\exp(-2\alpha L)}\right)x\right] \tag{10}$$

### 2.2 Discrete feature model for groundwater flow in fractured bedrock

The basic assumption of the discrete-fracture modelling approach is that groundwater flow in a 3-D space can be adequately represented in terms of a set of interconnecting transmissive, discrete features, each of which is essentially two-dimensional. This approach was applied in the performance assessment exercise called SITE-94. In this study, the rock beneath the island of Äspö, Sweden, was modelled by using the discrete-feature model which is defined within a 5 km × 5 km × 1 km domain (Geier, 1996a). The discrete-feature model is assembled from specifications for the following components:

1) large-scale hydrologic structures (fracture zones and extensive single fractures),
2) stochastic, discrete-fracture network (DFN) in the vicinity of the repository,
3) hydrologic connections due to the fractured, far-field rock mass and
4) man-made hydrologic features in repository, such as the disturbed-rock zone around repository tunnels and shafts.

The fully stochastic DFN model was applied based on statistical analysis of data from core, outcrops and packer test on Äspö for a 450 m × 320 m × 80 m block around the repositories (SKI, 1996). Further, macroscopic hydrological properties within each fracture is modelled either of two ways, by assuming either uniform or stochastic fracture apertures.

Advective-dispersive transport within the network model was represented by particle tracking with respect to steady-state solutions of the finite-element equations for the hydraulic head in the network model (Geier, 1996b). Thus, the expected value of the residence time PDF, $g(\tau)$, of inert water parcels travelling through fracture networks is obtained with help of Monte Carlo simulations of the flow field and particle tracking.

In SITE-94, the hydrological parameters associated with the macro-flow behaviour are translated into a hydraulic dispersion coefficient, E, and a flow velocity, u, and used in a one-dimensional model for solute transport. The coefficients E and u were estimated by fitting a one-dimensional advection/diffusion model to the $g(\tau)$ obtained from above mentioned simulations. For the simulation variant SKI0/NF0/BC0/HI in SITE-94, 10 realizations of the Monte Carlo simulations together with particle tracking were performed for obtaining the residence time PDF of released inert water parcels from a source which was randomly chosen from 40 sources/canisters. Fig. 1 shows the result of $g(\tau)$ with the release of inert water parcels from canister 2 from the first realisation of the network in the variant SKI0/NF0/BC0/HI.

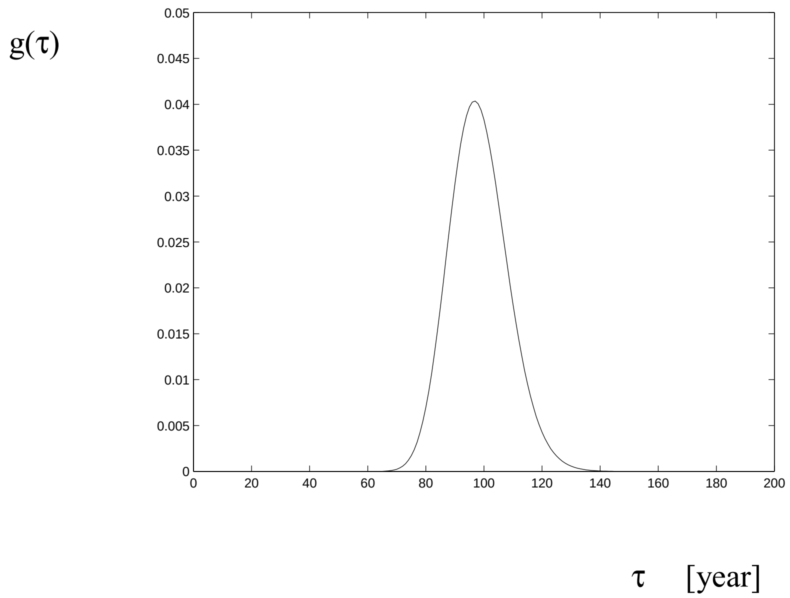


Fig. 1 The residence time PDF of inert water parcels from a single canister through the fracture network to the biosphere, in which x=500 m, u=5.14 m/y and E=4.21 $10^{-7}$ $m^2/s$.

## 4. Results and discussions

In SITE-94, radionuclides were assumed to escape from damaged canisters and migrate to the biosphere in a manner described in the section 2.2. The solute transport was estimated by using a 1-D transport model similar to (2) to (4) called CRYSTAL (Worgan and Robinsson, 1995) with the hydrological parameters obtained from the application of discrete-feature model. In this section, we compare the results of this 1-D approach with the convolution approach proposed here. The approach proposed here convolutes the 1-D transport model solution with the water flow in the fracture network corresponding to $g(\tau)$ in Fig. 1 according to (1). The function $f(t, \tau)$ is expressed by (10) normalised with its zeroth moment, $M_0$. The solutions of (8) and (11) in real time domain were obtained by using a numerical inversion algorithm (De Hoog et al., 1982).

Fig. 2 shows that there is a small difference between these two solutions in this simple demonstrative case. This is because the effect of the three dimensional nature of the flow is accounted for also in the 1-D approach in a simplified manner. The main difference between the two approaches lies in possibilities to account for complications not considered in the basic formulation. When the effect of heterogeneity in rock properties was accounted (Xu et al., 2001; Wörman et al., 2001), the difference between these two solutions is significant (see Fig. 2) even only the geostatistics of the rock properties for single fracture was used. The homogeneous case exhibits a more pronounced peak concentration than the heterogeneous case but the tail concentrations are particularly important for the estimation of the period of time during which a limiting concentration is exceeded.

The convolution approach has the advantages that the formulation is more flexible to include other processes and certain considerations not accounted for in (10). As an example for the safety analyses, it can be relevant to take into account spatial heterogeneity in rock properties, sorption kinetics and the impact of colloids. The convolution approach proposed here can more reliably include these effects in a three-dimensional fracture network than a simplified 1-D approach. Furthermore, the convolution approach opens for possibilities of expanding (10) in a series of terms representing the spatial distribution of radioactive doses on the ground surface and the biosphere. This feasibility is of utmost importance for risk assessments related to a leaking repository.

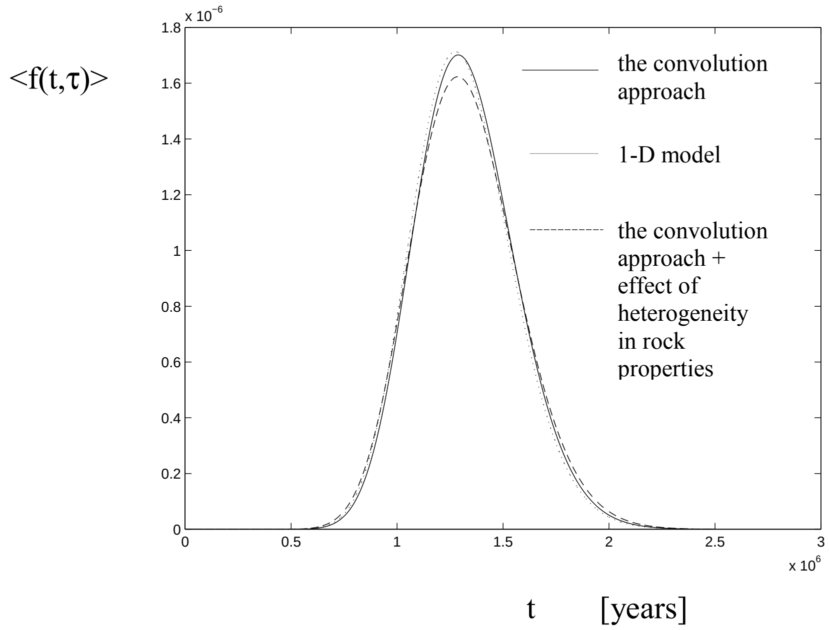


Fig. 2 A comparison of residence time PDF of solutes in water parcel versus time by using the 1-D transport model solution (9) and the travel time approach (1) in which f(t, τ) is expressed by (10). The following parameter values were used in the calculations: u=5.14 m/y, E=4.21 $10^{-7}$ $m^2/s$, $K_D$=54000, ε=0.005, Dp=$10^{-10}$ $m^2/s$, h=0.002 m and L=0.05 m.

# References


Cvetkovic, V., Selroos, J. O. and Cheng, H. (1999). Transport of Reactive Tracers in Rock Fractures. *J. Fluid Mech*. 378, 335-356.

Dagan, G. (1989). Flow and Transport in Porous Formations, *Springer-Verlag*, Berlin.

De Hoog, F.R., Knight, J.H., Stokes, A.N., 1982. An Improved Method for Numerical Inversion of Laplace Transforms, *J. Sci. Stat. Comput*., 3(3), 357-366.

Geier, J.E. (1996a). Discrete-feature Modelling of the Äspö Site: 2. Development of the Integrated Site-Scale Model (SITE-94), *SKI Report 96:6*, Swedish Nuclear Power Inspectorate, Stockholm.

Geier, J.E. (1996b). Discrete-Fracture Modelling of Äspö Site: 3. Predictions of Hydrogeological Parameters for Performance Assessment. (SITE-94) *SKI Report 96:7*. Swedish Nuclear Power Inspectorate, Stockholm, Sweden.

Grisak, G. E. and Pickens, J. F. (1980). Solute Transport Through Fractured Media 1. The Efect of Matrix Diffusion. *Water Resour. Res*. 16(4), 719-730.

Moreno, L., Tsang, Y. W., Tsang, C. F., Hale, F. V. and Neretnieks, I. (1988). Flow and Tracer Transport in a Single Fracture: A Stochastic Model and Its Relation to Some Field Observations. *Water Resour. Res*. 24(12), 2033-2048.

Neretnieks, I (1980). Diffusion in the Rock Matrix: An Important Factor in Radionuclide Retardation?, *Journal of Geophys. Res*., 85, 4379, 1980.

Painter, S. and Cvetkovic, V. (2001). Stochastic Analysis of Early Tracer Arrival in a Segmented Fracture Pathway. *Water Resour. Res*., 37(6), 1669-1680.

Rodriguez-Iturbe, I., Rinaldo, A. (1997). Fractal River Basins. *Cambridge University Press, Cambridge, United Kingdom*.
SKI SITE-94, Deep Repository Performance Assessment Project, *SKI Report 96:36*, Swedish Nuclear Power Inspectorate, Stockholm, Sweden.
Wels, C., Smith, L. and Vandergraaf, T. T. (1994). Influence of Specific Surface Area on Transport of Sorbing Solutes in Fractures: An Experimental Analysis. *Water Resour. Res*. 32, 1943-1954.
Worgan, K. and Robinsson, P. (1995). The CRYSTAL geosphere transport model: Technical documentation, version 2.1. *SKI Report 95:55*, Swedish Nuclear Power Inspectorate, Stockholm.
Wörman, A., Xu, S. and Dverstorp, B. (2001). Kinematic Analysis of Solute Mass Flows in Rock Fractures with Spatially Random Parameters. *Submitted to Journal of Contaminant Hydrology*.
Xu, S. and Wörman, A. (1999). Implications of Sorption Kinetics to Radionuclide Migration in Fractured Rock. *Water Resour. Res*. 35(11), 3429-3440.
Xu, S., Wörman, A. and Dverstorp, B. (2001). Heterogeneous Matrix Diffusion in Crystalline Rock – Implications for Geosphere Retardation of Migrating Radionuclides. *Journal of Contaminant Hydrology*, 47(2-4), 365-378.

# Plutonium and Neptunium Transport: Sorption Modeling for Performance Assessment of Nuclear Waste Disposal in the Fennoscandian Shield

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## Extended Abstract

Geochemical modeling with the USGS code PHREEQC was used to investigate thermodynamic and environmental uncertainties in performance assessments of potential Pu and Np migration in the crystalline rocks of the Fennoscandian shield. Sorption of Pu and Np was assumed the predominant cause of Pu and Np retardation during transport, and was modeled using a diffuse-double-layer-surface-complexation (DDLSC) model.

Uncertainties in the thermodynamic model were partially evaluated by comparing modeling results obtained with the NEA (HATCHES) Np and Pu aqueous thermodynamic database with results obtained using the EQ3/6 database. Due to a paucity of available data, all simulations used the same set of Np and Pu surface complexation constants (compiled by Turner, 1995).

"Batch" simulations were used to estimate Np and Pu partitioning and retardation factors under different environmental conditions. Various Np and Pu contaminated waters were considered: initially oxygenated glacial meltwaters, or alternatively, shallow dilute, intermediate, or deep saline waters collected near the Äspö HRL. Different sets of mineral assemblages, consisting of pyrite, FeS, calcite, goethite, or $Fe(OH)_3$ were used to buffer the aqueous chemistry of the Np- and Pu-contaminated glacial meltwaters. The non-linearity of the partitioning process was established 1) by varying the equilibrium Np and Pu aqueous concentrations from $10^{-8}$ to $10^{-11}$ m, the range of concentrations considered in the SITE-94 SKI project, and additionally 2) by comparing the equilibration of a fixed amount of sorption sites with an increasing number of water volumes (from a single one to an infinite amount). Uncertainties in any of the above factors were found to generate order of magnitude, and greater, differences in calculated Np and Pu partition coefficients. For example, differences in the contaminated waters and in the buffering-mineral assemblages chosen caused resultant Np and Pu partitioning coefficients to vary by up to 12 orders of magnitude, although the variation amongst coefficients with values greater than 1 (i.e. resulting in retardation factors of 2 or greater), was in the 3 order of magnitude range for Np and Pu aqueous concentrations fixed at $10^{-8}$ m, and up to 5 orders of magnitude for simulations using lower Np and Pu aqueous concentrations.

Uncertainties relating to the applicable temperature of the Np and Pu contaminated waters were also investigated and found relatively important in trying to determine/predict the applicable Pu partitioning coefficients (causing up to 1 order of magnitude differences in values greater than 1), but not as important in determining the Np partitioning coefficients. The effect of changing the amount of electrostatic charge by an order of magnitude, from 540 $m^2$ per kg of $H_20$ to 54 $m^2$ (without changing the number of sorption sites) was also investigated, but found relatively unimportant in the calculation of effective Np and Pu partitioning coefficients.

Pu partition coefficients calculated for Pu sorption from contaminated waters were generally much smaller than equivalent coefficients calculated for Pu desorption into initially uncontaminated waters. In contrast, Np partitioning coefficients were generally found to be greater for Np sorption than for Np desorption. Important differences in the redox behavior of Np and Pu, and the limited amount of thermodynamic information concerning the sorption of all the various Np and Pu redox states are in part responsible for these observations.

One-dimensional reactive transport simulations, using the PHREEQC code, investigated the potential retardation of Np and Pu transport, assuming a DDLSC sorption model, both during infiltration of Np- and Pu-contaminated waters and during clean-up of an Np- and Pu-contaminated environment. Simulations conducted using five different spatial distributions of sorption capacities, but with the same total sorption capacity, were compared to each other. In one case a uniform distribution was used. In three other cases, a spatially random log-normal distribution was used, appropriately scaled to standard deviations of 0.5, 1, and 2 log units. In a final case, the sorption capacities in the log-normal distribution with a standard deviation of 1 were spatially rearranged so that the one-dimensional distribution had an autocorrelation length of 8 m, rather than 2 m (in the initial case).

The results obtained from these transport simulations, differ markedly from those that could be obtained using more conventional modeling approaches, using a constant Kd sorption model or even a Langmuir or Freundlich isotherm model. Amongst the more important findings, the following stand out:

1) Partitioning coefficients vary non-linearly with increasing concentration, although effectively constant values were obtained in the case of the spatially uniform distribution of sorption capacities.

2) Effective partitioning coefficients describing radionuclide transport (by desorption) during the clean-up stage are likely to differ significantly from values applicable to transport during the infiltration stage. For example, the Pu desorption front was found to travel 5 times more slowly than the Pu sorption front.

3) Np and Pu aqueous concentrations obtained during "cleanup" of a contaminated environment can be more than an order of magnitude greater than the concentrations initially present in the contaminating waters, especially, but not only, if the radionuclide was strongly sorbed during infiltration of those waters,

4) Increasing the variance of the sorption capacity distribution results in an increase in the spreading of the breakthough curves for significantly sorbed constituents, and can mimic the effect of increasing the longitudinal dispersivity. Despite the relatively conservative behavior of Np, it's profile and breakthrough curves do not exhibit a simple gaussian shape, even in the case of the column with a uniform sorption capacity distribution. The breakthrough curves obtained for the end of the column document several trend reversals.

Reardon (1981) demonstrated the limits of applicability of the linear Kd concept for a one-dimensional system, under initially dynamically evolving conditions, and also under steady state conditions. The system assumed equilibrium ion-exchange reactions and slow calcite dissolution kinetics. The spatial variation in effective Kd values observed by Reardon under steady state conditions can largely be explained by his assumption of slow calcite dissolution kinetics.

In contrast to Reardon's simulations, the transport simulations presented here use the Local Equilibrium Assumption for all described reactions. Nevertheless, many of the radionuclide transport results obtained could still not be duplicated if commonly used sorption models, such as the constant Kd, Langmuir or Freundlich models, had been used instead of a DDLSC model. Transport simulations conducted using the DDLSC and other relatively complex multi-species models may 1) provide guidance in the appropriate use of simpler sorption models, and 2) may eventually provide minimum and maximum estimates of radionuclide retardation factors. The latter use, however, will be dependent on the availability of fairly complete and accurate thermodynamic data, describing not only aqueous speciation, but also surface complexation, and other heterogeneous reactions.

# Radionuclide Transport Modelling on new tools for regulatory purposes [2]

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## Abstract

In this summary we describe some recent work conducted at the Physics department of Stockholm University - Stockholm Centre of Physics, Astronomy and Biotechnology (SCFAB). We also suggest future developments of software tools that we think cover important aspects and pertinent needs for SKI and SSI in the few years to come as well as in the long term. The background is to be found in the well know fact that the work of SKB has entered in a new phase of development and demonstration which in turn may imply some shift in efforts towards the development of tools for assessment rather than research tools in order to fulfil the strategy of SKI and SSI in their regulatory work.

## 1. Probabilistic System Analysis- SYVAC/SU

During the Project-90 and SITE-94, the main tool used by SKI aimed at variability studies and probabilistic analyses of an hypothetical repository system for spent nuclear fuel was the SYVAC/SU code. This code allows to run some SKI models for simulation of the near-field and the geosphere releases in a probabilistic mode (Monte Carlo simulations) and obviously also in the deterministic mode if the user chooses to run a single realisation instead of say, thousand or ten thousand realisations. This code is a commando oriented code and it is not sufficiently flexible and user-friend according to modern requirements of flexibility, easy of use and transparency. Another clear weakness of this code is the fact that a significant amount of work is needed each time a new model is to be incorporate in the framework of SYVAC/SU.

- We recommend SKI to gradually phase out SYVAC/SU and substitute it by a modern window based tool for probabilistic system assessments which is:

- User-friendly
- forms an SKI standard, based on a "Lego approach" for software development.
- allows to couple in an easy way new codes as well as already developed codes, to the Monte Carlo driver.
- has a database with different models for the near-field, far-field (and simplified biosphere) which can be coupled to each other in chain at the will of the user, through a modern graphic interface.
- has a standardised output format

- We are presently coding some of theses ideas within the context of an SSI project. This work will be demonstrated at the workshop. But the code with the preliminary name of

[2] • – suggestion to new development
• – presentation of results at the workshop

ECOLEGO is only being developed for biosphere modelling. Nevertheless, using the same approach as in ECOLEGO it would be easy to implement a whole chain of models covering also the near-field and geosphere and making it a general purpose tool for the performance assessment. Our code is based on MatLab and allows therefore to couple to it submodels made in Matlab, C, $C^{++}$ and Fortran. The advantage of using this well know language for technical computing is the access to a whole library of numerical routines and tools which make it very fast to create new codes reducing significantly the time of development and hence the total cost. Part of the QA assurance is implicitly granted by the extensive tests already done on the MatLab libraries. Finally the easy to create a modern windows based system which can be tailored to be user-friend, also speaks for this approach for software development.

## 2. PSANA 2.0 - a general purpose tool for the post-processing of results from probabilistic assessments.

SKI has an own code for statistical post-processing of results obtained by SYVAC/SU, the PSANA code, that needs to be upgraded. The subroutines of this code made in Fortran are linked to two special graphic interface programs, GRAPHER and SURFER which are needed to display the pictures and statistics for analysis and reporting. The numerical subroutines are limited to some few standard statistical methods and therefore during these last years a commercial package, STATISTICA, has been used in parallel to PSANA for certain types of analyses because it is not motivated to develop own statistical routines from scratch. But this approach is in fact not effective nowadays.

- It is recommended that a modern and user-friend statistical post-processor for analysis of the performance assessment should be developed for use by SKI. It should include both the library of numerical subroutines and the graphics in an integrated fashion. Once again the use of MatLab with its impressive library for graphics and quality assured numerical and statistical tools will facilitate a very fast and cost-effective development of such an integrated analysis tool ( call it PSANA 2.0) for the performance assessment. To this tool one can add successively and very easily, new pieces of code that implement new methods and approaches for *uncertainty and sensitivity analyses* as they become necessary. Such a tool combines the flexibility of STATISTICA with the dedicated goal of PSANA.

## 3. Models for simulation of radionuclide transport in the near-field and geosphere.

For a decade ago, geosphere and biosphere models used in our field were considered quite advanced in relation to general ecological models of transport of chemical contaminants in the environment that were developed elsewhere at different laboratories and universities. Today the situation is being inverted: a scanning of literature in the field of environmental sciences can reveal for instance impressive studies of a whole bay mapped in three dimensions showing details of the circulation of contaminants and of their environmental impact. Obviously these are research models but confidence building requires the necessity to keep the state of the art of modelling radionuclide transport in parity with the advances in large scale modelling in the environmental field.

Assessment models for regulatory purposes differ from the research models mentioned above. The first ones are relatively simple and/or require a limited data set and the second ones are more complex and/or require more detailed input data. If the second group of models are aimed to a, as good as possible, understanding of important mechanisms behind phenomena that allow new theoretical insights, the first group is aimed at an easy and transparent overview of the repository performance and safety by making available (and condensing) a broad spectrum of scientific information needed for the process of decision making.

But the board between these two types of models moves in some way, continuously. The advances in computer technology and numerical modelling make it possible today, to use models that were considered too CPU-intensive for only some years ago (and almost by definition considered as research models) and at a significantly reduced price. One should take the advantage of this situation by continuing to move to "distributed models" in the assessments instead of using too simplified models. The main reason is transparency. In fact some of the models used today are very difficult to check because of the too many assumptions of "equivalent" processes needed to attain that degree of numerical simplification, which in the past was justified because otherwise the code behind those models should be very time consuming and therefore expensive.

So it is recommended that, for the sake of transparency of the peer review in a regulatory context, such "simplified" models should be substituted by (easy to grasp) physical formulations translated in clear systems of for instance differential equations, whenever possible and leaving the use of equivalencies and analogies to the places were they are really needed, for instance in the description of those processes for which data or knowledge is scarce. It should however be recognised that, for a considerable number of cases the (very) simplified assessment model is still the only way "out" of the problem. What we mean is that this way of introducing “equivalencies” should still be used but not become an “easy” practice whenever more transparency for the sake of the technical review process is possible.

- In the above mentioned context we think that SKI would consider as a medium term project the continued (see CALIBER) development of models in two or three dimensions which represent the physical geometry of canisters, tunnels, etc. in a more realistic way then what is possible with the presently used assessment models. Once again, fast PCs and the FEM (finite element) software today available will allow the development or alterations of such models within a reasonable time period. This will make SKI well prepared with an updated suite of models to meet the needs of coming reviews of SFL3-5 and of the spent nuclear fuel repository.

- A commercial finite element package is being used just now to model in 2D the near-field release from the tunnels of SFR (BTF1, BTF2, BMA and BLA) and some of the results will be shown during the workshop).

- SKI and SSI should also discuss if there is a need of a model for the biosphere-geosphere interface.

## 4. The probabilistic performance assessment

In GESAMAC project (“Conceptual and computational tools to tackle long-term risk from nuclear waste disposal in geosphere”) financed by the European Community, we have developed a parallel Monte Carlo driver (PMCD) for a parallel supercomputer. Some times it can be justified to use such a driver as was the case in that project because some unusual, although physically reasonable combination of parameters, made the assessment model to work with a too fine grid and therefore to consume too much CPU-time in the middle of a set of Monte Carlo simulations.

- The model used in the GESAMAC project was a transport model which including reaction kinetics. Some results related to the performance of a new version of the Parallel Monte Carlo Driver will be shown at the workshop.

Unfortunately the use of supercomputers is expensive and therefore as a continuation of that project we are now setting up our own "home supercomputer" a so called Beowulf for parallel computations. This will avoid the need to pay CPU-time to external providers of super-computer power. The Beowulf, which is made of a simple cluster of PC computers coupled to each other through a dedicated network has increased in popularity at universities as a cost--effective alternative to external supercomputer providers. With some 15 to 25 PCs in parallel one can get good supercomputer performances at "no price". Therefore avoiding probabilistic calculations is no more motivated by the argument of cost. In the majority of cases it is more clear to grasp the impact of uncertainties in the performance assessment by looking at the condensed results of the uncertainty and sensitivity analysis extracted from the M.C. calculations than to follow tens to hundreds of calculations of deterministic cases with the associated motivation for the parameters values used, assumptions for each case or why those cases were selected (or alternatively discarded). Finally one should recognise that even one single PC can nowadays be used to make standard Monte Carlo calculations for the performance assessment.

- A development that we claim is needed for the performance assessment addresses the issue of conceptual or model uncertainty. How much of the uncertainty is due to parameter uncertainty (and variability) and how much is due to model uncertainty? The standard way to estimate model uncertainty is to run different models and compare the results from each run. This is obvious for deterministic calculations. But for the probabilistic assessment there is today *no formal framework* to address the issue of parameter uncertainty combined with model uncertainty. In GESAMAC we studied a similar situation which was a *combination of parameter uncertainty with scenario uncertainty* (*model uncertainty was not addressed*) . We could show that for the suite of scenarios that were included in that project, the scenario uncertainty contributed to the total uncertainty with approximately 30%. But this result cannot be generalised, it is specific for the GESAMAC study. We think that addressing the combination “parameter uncertainty + model uncertainty” is more fruitful then “parameter uncertainty + scenario” uncertainty by reasons that we cannot develop here. Therefore we suggest SKI to consider this type of study.

# Quantitative Assessment of the Potential Significance of Colloids in Radioactive Waste Disposal Performance Assessment

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The primary objective of this project has been to evaluate the potential significance of colloids in performance assessment (PA) studies, with particular reference to the KBS-3 disposal concept. Colloids are minute particles in the size range 1 nm to 1 • m that can remain suspended in water. Groundwaters often contain significant populations of natural colloids, and these can interact with pollutants and influence their transport. In radioactive waste disposal systems, natural colloids and waste- and repository-derived colloids may influence radionuclide transport. Recent observations made by United States Department of Energy (DOE) researchers at the Nevada Test Site (NTS) have demonstrated migration of Pu 1.3 km from the site of the BENHAM underground nuclear tests, and suggest that the migration may have occurred owing to the attachment of the Pu to colloids.

Groundwaters sampled at the NTS ERDA 12 well cluster contain radioactive isotopes of Pu, Am, Cs, Co and Eu. The isotopic composition of the Pu observed at the ERDA 12 well cluster matches the composition of Pu from the BENHAM underground nuclear test, implying that the Pu has migrated 1.3 km in ~30 years.

At the sampling point, the radionuclides are associated with colloidal material in the groundwater. However, the identity of the colloidal material is uncertain. Cs, Co and Eu are probably associated with clays and zeolites, whereas Pu may be an intrinsic colloid. Ongoing US DOE research is seeking to determine the nature of the colloidal material.

It is not clear whether the Pu has been transported as colloids for the entire distance from the BENHAM shot point to the observation point. The mechanism of prompt injection has been observed to transport radioactive material outward from an underground nuclear test shot point at other NTS localities, but has never before been observed to operate on a scale greater than 300 metres. The high permeability of some volcanic units such as lava flows, and the perturbations to the regional hydrologic system caused by repeated underground nuclear testing, may be responsible for enhanced radionuclide transport.

The NTS observations suggest that Pu transport models taking into account only sorption and solubility may underestimate Pu migration potential. As a result of these observations, PAs for the Yucca Mountain Site have taken into account the potential for colloidal transport of actinides, and have used wide ranges of parameter values to assess the remaining uncertainty. The Yucca Mountain Viability Assessment (TSPA-VA) has included mechanistic models, and dose calculations for the transport of radionuclides by colloids involving both reversible and irreversible sorption.

The observations at the NTS are not directly applicable to the KBS-3 disposal concept. The following comparisons may be drawn:

- The mineralogy of the KBS-3 and NTS geological environments are similar. However, NTS rocks are finer grained and more heterogeneous in composition and texture.

- The KBS-3 and NTS hydrogeological environments are dominated by fracture flow. KBS-3 is assumed to be in a steady-state hydrological regime, whereas at the NTS, transient effects are caused by underground detonations.

- There is no major difference in the natural background colloid concentration, or the main colloid types at the NTS or in the KBS-3 concept.

- A key difference between the NTS and KBS-3 is the contrasting mode of emplacement of the radioactive material. In the KBS-3 disposal concept, the waste is emplaced passively, and is protected from the surrounding hydrogeological environment by an engineered barrier system. At the NTS, the radioactive source material was emplaced explosively, with attendant fracturing of the local country rock, and it was immediately exposed to flowing groundwater. In the KBS-3 disposal concept, the waste would only ever become directly exposed to groundwater after the engineered barriers were breached.

We have undertaken a quantitative assessment of the implications of the NTS observations for disposal system performance assessment in Sweden. We have also made a more general evaluation of the impact that colloid-facilitated radionuclide transport may have on the performance of the Swedish KBS-3 concept for disposal of high-level radioactive waste and spent fuel. These studies have involved the evaluation and application of SKI's colloid model, COLLAGE II, to the modelling of km-scale Pu transport at the Nevada Test Site (NTS), USA, and to the identification of circumstances under which colloid-facilitated transport could be important for a KBS-3-type environment.

Some modifications to the COLLAGE II code have been necessary in order to use it to model the NTS observations and to apply it to the KBS-3 disposal concept. The modelling had been complicated by the inflexible modelling timescales available in COLLAGE II. In order to simulate the migration of Pu at the NTS, COLLAGE II was modified to allow for user-defined timescales. The following input parameters were added to the input file:

- DELT: The timestep for explicit timestep specification.
- POW & TINC: For setting exponentially increasing timesteps.
- TFIN: To set the model simulation time.

A preliminary conceptual model of colloid-facilitated Pu transport at the NTS was developed. The model domain was conceptualised as a single fracture (a hypothetical extensional fault). The Pu was injected into the fracture equally distributed between mobile colloids and in solution. Two cases were modelled: irreversible (or very slow) sorption and reversible sorption onto colloids. The partition coefficient for binding of Pu to mobile colloids was varied by four orders of magnitude in both cases.

Two sets of models of Pu migration from the Benham Test were evaluated. One set had a high value for the rate at which radionuclides become sorbed or desorbed from mobile colloids (ALPHA1 = 52,560 $yr^{-1}$, which equates to 10 minutes for equilibrium to be reached). The other had a low value (ALPHA1 = $3 \times 10^{-2}$ $yr^{-1}$, which equates to 30 years for equilibrium to be reached). In each set the partition coefficient for Pu to free colloids (K1) was varied from 1 to 1000.

The results of the irreversible sorption models were all very similar with approximately one third of the inventory migrating 1.3 km, the same distance as apparently occurred at the NTS. Almost all of the Pu was attached to colloids. For the reversible sorption models the partition coefficient had a significant effect. For low values of the partition coefficient, the fluxes calculated were extremely small. For high values of the partition coefficient, significant fluxes were observed and about one fifth of the inventory migrated 1.3 km.

We have also conducted structured sensitivity studies aimed at identifying potential conditions (critical modelling assumptions and areas of parameter space) in which colloids have the potential to influence the results of repository performance assessment calculations for the KBS-3 concept.

The COLLAGE II model has been used to model colloidal radionuclide transport for the KBS-3 repository concept, using appropriate information on the characteristics of the sites considered in SR-97 (Aberg, Beberg and Ceberg). To constrain the scope of the task, a simplified representation of one of the SR-97 sites has been developed and appropriate sensitivity studies made around that representation.

The modelling is directed at identifying the parameter ranges for which radionuclide transport by colloids could be significant. The scenarios considered include all scenarios in which a radionuclide flux leaves the near-field, paying particular attention to situations in which colloid transport is likely to be significant, such as a case in which glaciation of the repository site causes an influx of relatively dilute waters into the groundwater system. Under these conditions the reduced salinity of the groundwaters leads to increased colloid stability and mobility as compared to the SR-97 analyses presented by SKB. Although the task has not extended to dose calculations, the sensitivity analyses help to address the question of how much greater the groundwater colloid concentration would have to be to have a significant impact on disposal system performance. Results so far indicate that under certain conditions, it is possible for colloids to have a significant effect on calculated disposal system performance, and that it is not possible to eliminate scenarios in which radionuclides are transported by colloids.

# Evaluating the Consequences of Uncertainty in Site Descriptions: A Discrete-Feature Approach

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Site characterization programmes are most often aimed at producing a single, "best" description of the main hydrogeologic features at a site. This description is then used as a basic framework for evaluating parametric uncertainties and the consequent risk of radionuclide release to the biosphere.

A hazard, especially in crystalline rock, is that important hydrologic features can be missed in the site description. This is especially true if the site characterization programme is focused on detailed characterization of a few features that were identified early in the course of the programme, or if the site investigations and interpretations are carried out by a single group of investigators, without an emphasis on fostering diverse interpretations.

Uncertainty regarding the basic framework of the site description is one of the more difficult aspects of system uncertainty to evaluate. One way to approach this problem is to evaluate the consequences of alternative, independent site descriptions.

In the SKI SITE-94 project, multiple site descriptions were evaluated by comparing distinct site models that were developed from the same data, by three independent institutions: the Swedish Nuclear Fuel and Waste Management Co. (SKB), the Swedish Nuclear Power Inspectorate (SKI), and the Swedish Radiation Protection Institute (SSI). The alternative descriptions were evaluated by the discrete-feature modelling technique, which proved to be flexible as a tool for assessing the effects of alternative site descriptions in terms of predicted distributions of groundwater travel times.

Results of this evaluation show that, for the specific site considered, the alternative interpretations did not lead to major differences in overall performance. However, this was largely because all three descriptions led to predictions of fairly direct paths for release to the biosphere, involving a few fracture zones that were relatively well characterized. At a site where more indirect paths for release are predicted, uncertainty in the site description could be of greater consequence.

In a review context, the question of uncertainty in the basic site description will still need to be addressed, especially if the geologic barrier function is a critical element of the safety case. The discrete-feature method is proposed as a relatively flexible method for evaluating alternative site descriptions, as well as for evaluating assumptions regarding the character of discrete transport pathways in crystalline rock. Ongoing developments in the modelling tools permit more advanced uses of this approach, including the prediction of transport path properties for Lagrangean models of radionuclide transport.

# The role of Biosphere Modelling in Radiation Protection from the regulator's perspective

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The authors will present their views on the role of biosphere modelling in SSI regulatory work in the field of Radiation Protection. The purpose and scope of the models, that might be relevant in different regulatory contexts, will be discussed. The presentation will focus on application of models for independent assessments of public exposure and exposure on the non-human biota and for obtaining derived standards suitable for risk assessments in different scenarios. The need for biosphere modelling in the field of waste management will be addressed in more detail. A strategy for SSI work in this field during the next five years will be outlined, including an analysis of the relationship between biosphere modelling and environmental monitoring.

# Geochemical Parameters Required from Site Characterisation

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## Introduction

This paper is being delivered at an interim stage of a review of geochemical parameter requirements that has been commissioned by SKI. In this paper, I start by discussing why this review is necessary and timely. This is followed by a categorisation and discussion of the uses for geochemical measurements in site characterisation by SKB and the corresponding evaluation by SKI. These categories of uses provide the basic framework for what will be done in site investigations and in the subsequent interpretations and modelling.

Uses of geochemical data for specific safety assessment purposes and through interpretative models for more general understanding of the geosphere environment and of its long-term evolution are well covered by existing SKB and SKI published papers and reports. These are of course supplemented by a vast literature on the geochemistry of proposed repository sites and underground laboratories in other countries, most notably those in fractured rock formations in Finland, Canada, Switzerland, France and England.

The purpose of this review is to examine from an objective and critical viewpoint the strategy that SKB is following and that will deliver information on which SKI will have to make regulatory decisions. A question particularly for SKI is whether these parameters will be representative, reliable and transparently appropriate for the safety requirements. In addition there is the additional question of whether the acquired parameters and interpretations will generate the desired level of confidence from review groups and the wider public. This paper offers some new ideas for discussion on the strategy, priorities and requirements for geochemical measurements from the regulator's perspective.

## Rationale for Reviewing Parameter Requirements

New ideas are justified and necessary because, for the first time in the crystalline rock repository programmes, sites are being characterised for selection and acceptance on the bases of open comparison of attributes and of safety. Not only will safe future performance be dependent on certain geochemical properties, but elimination of proposed sites may also be dependent on geochemical parameters or interpretation. Site evaluation and acceptance should be underpinned by demonstrable understanding of 'how the host geosphere system works', in a wider context than the narrow prescription for safety assessment. This means that data (geochemical data for the purpose of this paper) must satisfy the needs of conventional and 'state of the art' interpretation of chemical and hydraulic processes.

Another reason why new ideas or fresh approaches are required in implementing the data acquisition and evaluation is the necessity for transparency and demonstrability. The ability to communicate what is being done, why it is being done, and what the results signify, is paramount. Therefore I argue the case for simplicity rather than complexity. Building on what has been learned in the preceding research projects, the proposed principles for data collection are:

- o Use desk study at the outset to estimate parameters, to set-up hypotheses for what will be found, and to prognose difficulties in meeting requirements;
- o Limit the extent of the primary data requirements to achieve simplicity and transparency, and to reduce the scope for contention;
- o Design data acquisition to achieve specific levels of knowledge of the system;
- o Agree targets and criteria for data reliability that are realistic and achievable;
- o Understand the qualifications on data that may limit how they can be used by non-experts;
- o Tie in 'first level' interpretation directly with data collection so that the significance of data is evident at the time of measurement.

## Outputs and Uses of Data

Coming now to the categories and uses of geochemical parameters, the SKB position has been stated in a number of recent reports contributing to the development of the present site characterisation strategy. The 'Parameters Report' (Andersson et al., 1998) discusses data requirements in categories defined by the conventional branches of geoscience (hydrogeology, chemistry, etc). A detailed rationale for hydrogeological information and its uses is given. Geochemical information is described in terms of a chemical model of groundwater and of its interactions with minerals and repository materials. This model provides the chemical parameters that are of primary importance to safety assessment, specifically to canister corrosion, bentonite performance, fuel dissolution and solubilities, and radionuclide retention in the far field. These chemical parameters are listed in Tables 6-2 to 6-5 of the 'Parameters Report'.

In addition to the 'performance' parameters, the 'Parameters Report' also identifies a range of hydrochemical and environmental isotopic data that will contribute to geoscientific understanding of the system evolution, of solute transport, of water flow direction and ages, and of natural trace element geochemistry as a guide to radionuclide behaviour. The parameters list for this purpose is in Table 6-6 of the 'Parameters Report'.

The rationale for data requirements in the 'Parameters Report' also lies behind the SKB position on what properties of the rock and groundwater system can be used for siting and evaluation of sites. Essentially, the report on 'what is required from the rock' presents a set of suitability indicators and criteria (Andersson et al., 2000). It thus effectively prioritises the data requirements covered in the 'Parameters Report'. It also sensibly distinguishes between criteria that can be applied at the feasibility study, site investigation, and detailed characterisation stages of site selection and evaluation, depending on the extent of available knowledge at each stage. Requirements and preferences are identified, the former being prohibitive or 'show-stopper' criteria and the latter providing guidance to what are likely to be suitable conditions as indicated by a safety assessment. The hydrochemical suitability indicators are listed in Table 1. A geochemical context, or 'function analysis' is also identified – this is essentially a rationale or model for the particular indicator parameter and in some cases identifies sets of additional parameters that support a 'more precise definition' of the indicator. Two observations can be made: firstly, that dissolved oxygen ($DO_2$) concentrations *per se* are absent from lists in both reports, and, secondly, that the absolute requirements are somewhat modified. For example, the 'Requirements Report' asserts that if none of the Eh indicators can clearly demonstrate the absence of dissolved oxygen, a deeper chemical assessment is required. In other words there remains some doubt about measuring this key requirement reliably.

**Table 1.** Suitability indicators for groundwater compositions, to be applied at the site investigation stage (from Andersson et al. 2000)

| Parameter | Requirement (Req) or Preference (Pref) | Criteria in Site Investigation |
|---|---|---|
| Dissolved $O_2$ | Req: Absence at repository level (indicated by negative Eh, occurrence of $Fe^{2+}$ and/or $HS^-$) | At least one of Eh, $Fe^{2+}$ or $HS^-$ must be satisfied |
| pH | Pref: Undisturbed groundwater at repository level should have pH between 6-10 | Values should be in range 6-10 below – 100m depth |
| TDS | Req: TDS <100 g/l | Values at repository level must be <100 g/l. Occasional higher values OK if located in areas that can be avoided |
| Others | Pref: DOC <20 mg/l<br>Pref: Colloids <0.5 mg/l<br>Pref: Low $NH_4$<br>Pref: $Ca^{2+}$+$Mg^{2+}$ > 4 mg/l at rep. depth<br>Pref: Low Rn and Ra | Attention to deviations from preferred concentrations |

## Assessing the Adequacy of Data for Required Parameters

I am proposing a slightly different approach to setting parameter requirements, to demonstrating the adequacy of data in terms of reliability and significance, and to building confidence in the robustness of both data and understanding. The essence of my proposal is that the requirements should focus even more strongly on establishing the adequacy of individual suitability and safety indicators. Another way of viewing this proposal is that the sampling and analysis classes that guide SKB's data acquisition strategy (see Section 9.5 in SKB 1998, and also Table B-6, SKB 2000) should be modified to ensure as an absolute priority that data for these indicators are demonstrably adequate and easily understood. Otherwise there is a possibility that although lots of data would be collected, none would specifically meet these primary requirements.

The revised requirements are best illustrated for discussion by taking in turn the two key suitability indicators: dissolved oxygen ($DO_2$) and salinity (TDS), and showing how the credibility and adequacy of data and understanding should be enhanced.

**Dissolved Oxygen ($DO_2$)**

The requirement is to show that $DO_2$ is absent at repository level. At present, SKB intend to meet this by showing that at least one of the proxy indicators Eh, $Fe^{2+}$ or $HS^-$ is indicative of absent $DO_2$ (Table 2). This, coupled with the 'let out' mentioned above for the case where none of the indicators could be established reliably, is arguably too weak a requirement. The requirement must be to demonstrate that data for $DO_2$ and other redox indicators give consistent and indisputable evidence to meet the requirement and also to understand the relevant geochemical system which accounts for this property (this is similar to the 'function analysis' of Andersson et al. 2000). This means that all of the indicators should be measured, should be shown with a geochemical model to be internally consistent, and that their evolution should be understood. The most robust way to approach this with respect to conditions at repository depth would be to make measurements systematically from the surface (i.e. from an environment which is known to be oxygenated).

The technical difficulty of establishing 'zero' or absent $DO_2$ would be met by demonstrating a trend of diminishing $DO_2$ and decreasing Eh with increasing depth. This approach has already been demonstrated for groundwaters in the Whiteshell Research Area in Canada (Gascoyne, 1997) and also to some extent in the Redox Zone Experiment at Äspö (Banwart et al., 1994). However data in Gascoyne (1997) also suggest that $DO_2$ may be detectable when the Eh is negative: there is one case of 80 µg/L $DO_2$ alongside Eh -75 mV, and general occurrence of 2-4 µg/L $DO_2$ corresponding to Eh <-90 mV. These highlight the potential contention that could arise if SKB were to follow the present strategy. A proposed revision to the data requirement is summarised as:

- $DO_2$, Eh and redox indicator species from surface to repository depth (both vertically and along flowpath to repository location);
- Geochemical calculations demonstrating that redox indicators consistently support the absence of $DO_2$ at repository depth and also support a model that $DO_2$ is eliminated during transport to repository depth.

The findings in Banwart et al. (1994) and Gascoyne (1997) suggest that dissolved uranium (U) and Dissolved Organic Carbon (DOC) should be included as measured redox indicators. The implication of these requirements for site investigation strategy might be to place more weight on a specific investigation to achieve these targets, in place of general data acquisition as suggested in SKB (2000 & 2001). Moreover the sensitivity of these parameters to perturbation indicates that measurements should be carried out at an early stage of site investigation, probably in purpose-drilled boreholes at a variety of depths, starting shallow and progressing to greater depths.

**Salinity (TDS)**

The requirement is to show that TDS at repository level is <100 g/L, although there is also a 'let out' for occasional higher values that are in avoidable locations. Unlike $DO_2$, this requirement does not present an analytical difficulty but it does raise an issue of what spatial density of data is adequate to be indisputable. An assessment of this issue requires a conceptual model of the present flow system, structural geometry and groundwater history ('palaeohydrogeology') that control salinity distribution. It also requires an expert judgement based on existing observations in similar systems, identifying where there might be sharp salinity transitions and sources of higher salinity. It is worth noting that this same conceptual approach and expert judgement is necessary for deciding how much hydrochemical data are required to establish in adequate detail the initial and boundary compositions that would feed into the use of hydrochemistry to test a groundwater flow model (as developed by Task 5 of the Äspö Groundwater Modelling International Task Force). The adequacy and credibility of work to meet this requirement would be well demonstrated by the following procedure:

- Construct conceptual model of salinity distribution, based on structure, inferred flow system, and regional geochemistry and hydrochemistry;
- Use conceptual model and observations in similar systems to predict salinity variations and maxima through system extending along flow paths towards repository location;
- Design borehole investigations to test predictions especially with respect to scales of variation and confirmation of maximum salinity;
- Use statistical testing to assess significance of variation from prediction, add data where necessary to improve confidence.

## Data Requirements for Scientific Understanding

Scientific understanding of a site, especially of how groundwater flows and solutes are transported, underpins the credibility of the case for geological disposal. The ease with which the groundwater system at a site can be understood and the flow model can be demonstrated to be a reasonable representation will be a major factor in building confidence in site suitability. It may be the dominant factor in site selection by SKB and in site evaluation by SKI. Therefore data requirements for scientific understanding are important though they do not rate as 'essential' for safety assessment.

**Identification of Groundwater Masses by Statistical Analysis of Hydrochemical Data**

Hydrochemical data are required for identifying volumes of groundwaters that have distinct compositions that are indicative of specific origins, flow directions and recharge ages. These data are palaeohydrogeological tools, and contribute to qualitative understanding of how the system evolved to its present state and how rapidly the system changes in response to external effects. A more quantitative use of the data is possible if there are sufficient hydrochemical contrasts in the system, i.e. distinct water masses, and sufficient independent knowledge of palaeohydrogeology that the data can be used to test a hydrodynamic model of flow, mixing and solute transport. SKB proposes to integrate hydrochemical data with the groundwater model by using a statistical analysis of the data to identify distinct groundwater masses and mixing between these masses (Laaksoharju, 1999).

Hydrochemical data requirements for this sort of approach are intensive, since a palaeohydrogeological reconstruction depends on inferred initial and boundary water compositions and measured data for spatial variation of present-day compositions. Moreover, if a future phase of site characterisation were to involve a transient drawdown experiment (i.e. a long-term pumping test or transport modelling in flow towards an underground excavation), then the present-day compositions data are the initial and boundary conditions for that model. In summary, if it is intended to couple hydrochemistry with flow modelling in this way, then a reliable increase in confidence is possible only with fairly intensive and systematic data acquisition along potential flow paths. The essentially-stagnant state of a low permeability flow system in its undisturbed condition means that groundwater compositions may change over small distances. [This also applies to the data requirements for ensuring that total salinity is everywhere below the suitability criterion of 100g/L].

## Estimating Groundwater Travel Times and Solute Residence Times

A related mode of hydrochemical data interpretation is the estimation of travel times, which mostly involves environmental isotope data. Travel times obtained from these data are for transport of the isotopic species as solutes through particular segments of the groundwater system. Typically they will be travel times from recharge to the point of sampling. This information is not directly comparable with hydrodynamic travel times that might be calculated with the groundwater flow model for the safety assessment; in this case the travel time typically applies to unretarded solute movement from repository location to discharge at surface. However there is a degree of useful comparability between the isotopic travel time and the assessment travel time that, in some conditions, would increase confidence in the flow model. Thus the specific data requirements for isotopic travel time estimation are an important consideration.

However it is widely recognised that interpreting travel times (or 'residence times') from isotopic data for deep groundwaters in such systems has large uncertainties. The appropriate long-lived environmental isotopes have uncertainties due to water-rock reaction ($^{14}C$, $^{234}U/^{238}U$), in situ production ($^{36}Cl$), and tough demands on sampling and analytical capabilities ($^{81}Kr$). Thus a 'data requirement' on its own is an inadequate strategy. The 'requirement', rather than just raw data, is an increase in understanding of rates of groundwater and solute movement through the system.

I propose that the initial requirement should be for knowledge of travel times in the shallower groundwater system, i.e. above repository depth – typically down to 100-200 metres depth. This knowledge is important on its own for understanding the geosphere-biosphere interface especially if it helps to identify recharge and discharge areas. It is also a logical first step in using isotopes to investigate the deeper system. Applying the theme of simplicity, I suggest that some straightforward requirements are:

- Depths to which detectable tritium ($^{3}H$) occurs in the undisturbed site (detection limit 0.1 tritium units TU);
- Depths to which detectable carbon-14 ($^{14}C$) occurs in the undisturbed site (detection limit 0.1 percent modern carbon pmc);
- Interpreted $^{14}C$ ages of TIC and TOC in groundwater in the main flow paths at representative depths, for example 100, 200, 300 metres;
- Stable oxygen and hydrogen isotope ratios ($^{18}O/^{16}O$, $^{2}H/^{1}H$), chlorine-36 ($^{36}Cl$) and radiogenic helium contents ($^{4}He$) at these depths.

These requirements focus effort on achieving a meaningful outcome. The present SKB strategy in the 'Parameters Report' and in the Geoscientific Programme for Site Investigation (SKB 2000) would acquire lots of isotope data for Class 5 samples but lacks a plan to maximise knowledge of groundwater travel times.

An important aspect of analysing for isotopic data is the very high sensitivity of data to sampling contamination (Nirex, 1997a, 1997b). Thus data requirements should specify that the best possible precautions should be taken to minimise and control contamination, e.g. through the drilling methods and use of tracers and by using dedicated boreholes in water volumes undisturbed by hydraulic testing, and to optimise the analytical detection limits and precision (as indicated above), i.e. by use of state-of-the-art facilities.

## Conclusion

This review of geochemical parameter requirements will recommend that geochemical parameter requirements should be linked with a requirement to show increasing knowledge of the groundwater system. This would mean that the acceptability of geochemical parameters would be assessed in terms both of the validity of key parameters, for example where these are essential safety requirements, and of an understanding of the relevant part of the groundwater system. Effort should be directed into data acquisition for a number of discrete tasks, such as dissolved oxygen decay in the shallow part of the system, heterogeneity of salinity and distribution of groundwater masses, and groundwater travel times and solute residence times. For many of these aims, parameter measurements need to be focused on the shallower parts of the groundwater system. Geochemical processes in this part of the system have to be understood as a precursor for the more difficult task of understanding the processes at repository depth. It is recommended that SKI should frame their requirements in terms of a number of straightforward objectives and not merely as an exhaustive data compilation. Such a compilation could become detached from the data quality, data density and interpretative requirements of a robust site evaluation exercise by SKI.

## References

Andersson, J, Almén, K-A, Ericsson, L O, Fredriksson, A, Karlsson, F, Stanfors, R and Ström, A. 1998. Parameters of importance to determine during geoscientific site investigation. Technical Report TR-98-02. SKB Stockholm.

Andersson, J, Ström, A, Svemar, C, Almén, K-A, and Ericsson, L O. 2000. What requirements does the KBS-3 repository make on the host rock? Technical Report TR-00-12, SKB Stockholm.

Banwart, S, Gustafsson, E, Laaksoharju, M, Nilsson, A-C, Tullborg, E-L and Wallin, B. 1994. Large-scale intrusion of shallow water into a vertical fracture zone in crystalline rock: Initial hydrochemical perturbation during tunnel construction at the Äspö hard Rock Laboratory, southeastern Sweden. Water Resources Research, Vol. 30, pp 1747-1763.

Gascoyne, M. 1997. Evolution of redox conditions and groundwater composition in recharge-discharge environments on the Canadian Shield. Hydrogeology Journal, Vol. 5, No 3, pp 4-18.

Geier, J, Tirén, S, Dverstorp, B and Glynn, P. 1996. SITE-94: site-specific base data for the Performance Assessment. SKI Report 96:10. SKI Stockholm.

Glynn, P D and Voss, C I. 1999. SITE-94: Geochemical characterization of Simpevarp ground waters near the Äspö Hard Rock Laboratory. SKI Report 96:29. SKI Stockholm.

Laaksoharju, M. 1999. Groundwater characterisation and modelling: problems, facts and possibilities. Technical Report TR-99-42. SKB Stockholm.

Nirex 1996. Rock Characterisation Facility, Longlands Farm, West Cumbria: Report on Baseline Groundwater Pressures and Hydrochemistry. Report No. SA/96/006. UK Nirex, Harwell.

Nirex 1997a. The Hydrochemistry of Sellafield: 1997 Update. Report No. SA/97/089. UK Nirex, Harwell.

Nirex 1997b. Evaluation and Interpretation of Carbon Isotope and Tritium Data for Groundwater Samples from Deep Boreholes at Sellafield. Report No. SA/97/094. UK Nirex, Harwell.

SKB 2000. Geoscientific programme for investigation and evaluation of sites for the deep repository. Technical Report TR-00-20. SKB Stockholm.

SKB 2001. Platsundersökningar: Undersökningsmetoder och generellt genomförandeprogram (Site investigation: investigation methods and general characterisation programme). Report R-01-10. SKB Stockholm.