Radioactive Waste Management

Linkage of Geoscientific Arguments and Evidence in Supporting the Safety Case

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FOREWORD

The long-term safety of a deep geological repository for radioactive waste will be strongly dependent on the performance of the geosphere. The geosphere potentially isolates the radioactive waste from possible future intrusions by humans; provides a stable physical and chemical environment for the engineered barriers within the repository, insulating against external perturbations such as earthquakes and climate change; and prevents, delays and attenuates radionuclide transport by virtue of its hydraulic and sorptive properties.

A safety case for a deep geological repository typically makes use of geoscientific information within a long-term safety assessment that evaluates potential impacts. These studies require a conceptual model of the geosphere that quantifies, for instance, groundwater flow rates and consequent radionuclide transport. However, geoscientific information can play a larger role in the safety case. In particular, geoscience can offer multiple and independent lines of evidence (qualitative and quantitative) to support a safety case. Moreover, geoscience can play an important role in other repository activities that bear on safety, such as site selection and repository design.

AMIGO, an OECD/NEA international project on Approaches and Methods for Integrating Geological Information in the Safety Case, brings together geoscientists from across the international community, most of whom are involved in studies on deep geological repositories. AMIGO is organised as a series of biennial workshops with sessions that include comprehensive technical presentations from the host organisation, plenary discussions on topical issues, and small group discussions concentrating on specific questions. Each of these sessions has a single unifying goal: to enhance the role of geoscience in the safety case. The AMIGO workshops generally focus on improving the use of geoscientific information in the safety case, and more specifically on:

- the role of the geosphere and its representation in the safety case;
- capabilities of site characterisation versus the needs of safety assessment modelling and the safety case; and
- procedures that encourage integration of a wide range of geoscientific information to contribute to the safety case more effectively.

The first AMIGO workshop (AMIGO-1) was held in Yverdon-les-Bains, Switzerland in June 2003, and was hosted by the Swiss National Co-operative for the Disposal of Radioactive Waste (Nagra), the Swiss Federal Nuclear Safety Inspectorate (HSK) and the University of Bern. Amongst the topics investigated was the use of multiple lines of evidence to build confidence in the geoscientific understanding that underlies the safety case.

These proceedings present the outcomes of the second AMIGO workshop (AMIGO-2), held in Toronto, Canada in September 2005 and hosted by Ontario Power Generation (OPG) and the Canadian Nuclear Safety Commission (CNSC). This second workshop expanded upon the AMIGO-1 deliberations to examine how geoscientific arguments and evidence are linked in supporting a safety case. It also examined the extrapolation and transfer of geoscientific information in time and space, and the practicalities of collecting, linking and communicating this information.

Acknowledgements

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Special thanks are also expressed to the following individuals:

- Members of the AMIGO Steering Group,[1] who were responsible for the management of the AMIGO workshop series as a whole, and who set the general objectives for this and the first AMIGO workshops.
- Members of the Scientific Programme Committee,[2] who were responsible for the detailed planning of this second AMIGO workshop, and who defined the lists of issues to be considered during the plenary and working group presentations.
- The working group chairpersons and rapporteurs, who led and summarised the debates that took place in the four working groups, and who presented their observations during the final plenary discussion.
- The speakers for their interesting and stimulating presentations, and all participants for their active and constructive contributions.

These proceedings drew from presentations made at the workshop, including introductory comments by Rick Beauheim, a summary of the AMIGO-1 workshop by Andreas Gautschi, summary comments by the session chair- and co-chairpersons, reports crafted by the working group rapporteurs with the assistance of the group chairperson and participants, and concluding remarks by Johan Andersson. The draft proceedings were prepared by Bruce Goodwin and Mark Jensen and reviewed by members of the Steering Group and the Scientific Programme Committee.

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1. INTRODUCTION

1.1 AMIGO and its objectives

The OECD/NEA Integration Group for the Safety Case (IGSC) is a technical advisory body to the OECD/NEA Radioactive Waste Management Committee. The IGSC brings together national programmes that are investigating the deep geological disposal of long-lived and high-level radioactive waste, and its focus is on the science and technology underlying long-term repository safety and on methods to improve confidence in repository safety cases. A repository "safety case" is defined as a synthesis of evidence, analyses and arguments that quantify and substantiate a claim that the repository is safe. It typically provides a comprehensive and specialised assessment of the expected long-term safety and potential impacts of a radioactive waste repository.

For deep geological disposal, studies of the geosphere form a principal component of the safety case. Accordingly, the IGSC has sponsored the AMIGO programme (NEA, 2003), an OECD/NEA international project on Approaches and Methods for Integrating Geological Information in the Safety Case. AMIGO is concerned with the collection and integration of geoscience evidence, analyses and arguments that contribute to an understanding of long-term safety.

Geoscience information is unique in that it can offer lines of reasoning that span millennia. It may involve diverse information from many sub-disciplines, such as geophysics, hydrogeology, geochemistry and paleohydrogeology. Another important characteristic of geoscience information is how it evolves over time. During the initial stages of planning for a repository, geoscience information may be limited and provisional, primarily because data are often sparse. The safety case will likely also be limited and somewhat uncertain. However, more data will be collected during subsequent stages such as repository siting and construction, and the iterative improvements will lead to a better understanding of the geosphere and its evolution, contributing to more convincing safety cases. If enough data become available, and the geoscience (and other) information is sufficient, the safety case may support a decision to proceed to an operational stage and, eventually, to closure of the disposal facility.

The objectives of the AMIGO project are (NEA 2003):

- to understand the state of the art and identify means to improve the ways in which safety cases are supported by geological information;
- to contribute to the development of methods for representing the geosphere in safety cases;
- to define terminology for communication and interaction between groups engaged in site characterisation and safety assessment in support of safety cases;
- to clarify the role and application of geoscientific information and evidence applied in safety cases;
- to clarify the relationship between and information requirements for site characterisation and safety assessment modelling; and

- to foster information exchange between international radioactive waste management geoscience programmes, and between academic, regulatory and implementing bodies.

AMIGO is structured as a series of workshops. The first workshop, AMIGO-1, was held at Yverdon-les-Bains, Switzerland, on 3-5 June 2003, and hosted by the Swiss National Cooperative for the Disposal of Radioactive Waste (Nagra), the Swiss Federal Nuclear Safety Inspectorate (HSK) and the University of Bern. It is briefly recapped in the following section. The remainder of this report summarises the second workshop, AMIGO-2, which was held in Toronto, Canada in September 2005 and hosted by Ontario Power Generation (OPG) and the Canadian Nuclear Safety Commission (CNSC).

1.2 Summary of the AMIGO-1 workshop

The AMIGO-1 workshop was focused on building confidence using multiple lines of evidence. It also examined, to lesser degrees, topics such as the role of the geosphere in the disposal concept, the use of geological information in waste management programmes, the synthesis of geological information, and integrating the work of geoscientists and safety assessors (NEA, 2004).

AMIGO-1 was broken into four main sessions. The first session concentrated on studies recently completed in Switzerland by the Swiss National Cooperative for the Disposal of Radioactive Waste (Nagra) and the Swiss Federal Nuclear Safety Inspectorate (HSK). Six presentations from Nagra provided a wealth of detail on their geoscience studies that concerned the (possible future) disposal of spent fuel, high-level vitrified waste and long-lived intermediate-level waste in the Opalinus Clay formation of northeast Switzerland. A follow-up presentation from HSK provided regulatory comments on this safety case. Many elements of these presentations found their way into the deliberations of the three working groups.

The second session of AMIGO-1 consisted of invited keynote talks from researchers in related fields, but outside the field of radioactive waste management. Two presentations, from P.H. Nadeau and L.A. Yose, covered studies in the petroleum industry and a third presentation, from S. Violette and others, dealt with diagenetic and hydrogeologic modelling of the Paris Basin. These presentations served to present (for example) new and innovative geophysical techniques and methods to manage large geological datasets from multiple sources, developed for the hydrocarbon industry but with potential applications in radioactive waste management programmes.

The third session was set aside for contributions of safety cases and associated studies being undertaken by other national organisations. It included oral and poster presentations by researchers from Belgium, Canada, France, Germany, Japan, Spain, Sweden, the United Kingdom and the United States. It became clear that the various national organisations are at different stages of study, ranging from licensing to site selection to feasibility studies, and that their level of geoscience understanding also varies and may have different short-term goals. The AMIGO workshops are seen to be important in sharing experiences and showing the path forward for geoscience studies.

The fourth session was devoted to smaller, parallel group discussions within three Working Groups and was followed by a plenary meeting to discuss the findings of each group:

- **Working Group A: Role(s) of the geosphere in the safety case**. This Group concluded “a convincing safety case requires (and geological characterisation aims to achieve) a good general scientific understanding of the geosphere, its evolution and its interaction with the repository” and “the development of the safety case proceeds iteratively with site characterisation, and interdisciplinary communication is of key importance to the success of both" (NEA, 2004).

- **Working Group B: Multiple lines of evidence involved in safety case arguments**. This Group observed that "multiple lines of evidence are used throughout the process of making a Safety Case" and generated a table of potentially applicable arguments, categorised by their value to support isolation, their effectiveness as a barrier to radionuclide transport, or their influence on long-term stability and predictability (NEA, 2004). These arguments are seen to be essential in supporting key conclusions made in the safety case, particularly concerning the potential performance of the geosphere.
- **Working Group C: Practical guidelines for managing the interaction between different teams involved with building a safety case**. The discussions and conclusions of this Group were summarised in six "practical management elements or guidelines":
  - communication between different stakeholders,
  - the need for and challenge of multi-disciplinary teams,
  - characteristics of a geosynthesis document,
  - encouragement and justification of geoscience efforts to address safety issues better,
  - the value of international consensus, and
  - similar experience in other geoscience programmes such as the petroleum industry and academia (NEA, 2004).

Practical experience in various national programmes discussed in these working groups were important motivators for the planned AMIGO compendium (see Section 4).

1.3 Structure of AMIGO-2 and outline of this report

The overall objective of AMIGO-2 was to examine the linkage of geoscience information and evidence used to create a unified and consistent description of the geosphere ("geosynthesis") that might be used to support a safety case. This objective is consistent with the goals of AMIGO, and in fact carries on from discussions that occurred at the AMIGO-1 workshop.

The structure of the AMIGO-2 workshop was slightly modified, compared with AMIGO-1, primarily to permit more time for discussion within the working groups. The agenda consisted of three main sessions:

1. The first session was set aside for presentations from the host organisations. It included four talks by OPG on geoscience research undertaken within the Canadian Deep Geologic Repository Technology Program. A fifth talk by the CNSC was concerned with geoscience and related topics in a forthcoming Canadian regulatory guide for assessing the long-term safety of radioactive waste management.
2. The second session involved invited presentations on four selected "key" topics: potentials and limits of the use of geohistory to understand current features and conditions and possible future evolutions; transferability of data and information from other sites (repository sites, natural analogues and generic underground research laboratories); potentials and limits of the collection of geoscientific data and information for characterising a site; and requirements for documentation of geoscientific data and understanding used to characterise a repository site (geosynthesis) and to support development of the safety case and its communication.

The authors of these presentations were asked to direct their attention to specific questions generated by members of the AMIGO Steering Group and Scientific Programme Committee, and to include (where possible) observations from other national programmes. Each presentation had multiple authors to help increase the breadth of the talks.

3. Session three centered on the deliberations of four Working Groups and occupied most of the second and third days of the workshop. There were four parallel Group meetings, four scheduled breaks for plenary presentations and a final plenary discussion. The first two breaks were devoted to the two invited keynote presentations: one on a new research project on the geological sequestration of CO_2 (S. Whittaker) and the second describing the current status of the OECD/NEA Clay Club (M. Mazurek). The third and fourth breaks were taken up with a discussion of the questionnaire for the AMIGO compendium (see Section 4) and a presentation on the optional field trip following the end of the workshop. These meetings and breaks were followed by presentation and discussion of the Groups' findings at a plenary meeting. The Working Group topics were:

   - geoscience indicators for safety (Working Group A),
   - communication of geoscience safety arguments (Working Group B),
   - realities of site investigation (Working Group C); and
   - assembly and integration of geoscience knowledge and arguments (Working Group D).

Section 2 of this report outlines the contents of the first two sessions for the host and key topics presentations. It also summarises the plenary discussions that followed. These sessions occupied the first day of the workshop and were followed, on days 2 and 3, by the Working Group discussions. Section 3 of this report summarises the results and plenary discussions that arose from the Working Groups. Section 4 presents a summary of the AMIGO plans for a geoscience compendium, taken from a special presentation made on the final day of the workshop. Finally, Section 5 includes general observations, conclusions and recommendations arising largely from the plenary presentations and discussions.

Part A of this report reproduces the written summaries of the four Working Groups. These summaries were prepared by the chairpersons and rapporteurs and approved by the Group members. Part B contains copies of the plenary presentations made during Sessions I and II and the presentations made within the Working Groups. The workshop participants are identified in the Appendix.

2. SUMMARY OF HOST AND KEY TOPICS PRESENTATIONS

2.1 OPG and CNSC presentations

Session I started with an overview of Canadian geoscience studies being performed under Ontario Power Generation's Deep Geological Repository Technology Program (M. Jensen). These studies are aimed at challenges common to most other national programmes:

- Develop field and laboratory tools to improve site characterisation capabilities and foster multi-disciplinary collaboration. These tools will also lead to an improved assembly and integration of information describing the role of the geosphere in the safety case.
- Evaluate and refine methods to characterise and quantify descriptions of the geosphere, especially directed at issues that involve uncertainty in spatial and temporal boundary conditions. One of the more challenging uncertainty issues is non-uniqueness, or divergent explanations that are consistent with observed data. These methods will lead to a clearer and more constrained understanding of parameter data, scenarios and geosphere models.
- Improve upon documentation at all levels. It is important to build confidence amongst geoscientists, and it is equally important to recognise that lines of communication must be established to other stakeholders. Better methods of visualisation are required to help with communication of complexities in the geosphere.

A key element in the programme is the development and demonstration of geoscience methods to aid in the creation of an integrated and site-specific descriptive conceptual model(s) within a Shield setting. As part of this approach, efforts have been focused on preparing multi-disciplinary case studies of deep-seated Shield groundwater flow system evolution at timeframes relevant for radioactive waste management purposes. This work programme, which involves the coordinated effort of 20 different groups drawn from universities, industry and government, provides a "workbench" to explore how results from different disciplines can be effectively integrated and linked. The case studies examine issues such as the factors affecting Shield flow system stability, and uncertainty in flow system history resulting from practical limitations in field site characterisation. Specific issues relevant to a deep geological repository assess the influence of uncertain fracture network geometry and interconnectivity, flow system perturbations by long-term climate change (temporal and spatial surface boundary conditions), permafrost generation and decay, glacial melt water recharge, and variable saline flow domains on flow system hydrodynamics and spatial groundwater compositions. This work has significantly benefited from the application of Virtual Reality tools that foster inter-discipline communication and the ability to explain the linkage of all relevant observations and data supporting geoscience knowledge of far-field barrier performance and resilience to change. The next three presentations provided an illustration of this approach.

A deep geological repository in Canada, and in many other countries, will be subject to episodes of glaciation and associated climate change, with consequent implications on safety. The second presentation (R. Peltier) in the host session described studies to understand potential impacts of continental glaciation and deglaciation caused by small variations in the Sun's thermal energy reaching the Earth. The goal is to develop constrained predictions of the duration and rate of change of glacial effects in the past, with extension to future changes on a hypothetical repository. Analyses of a North American glacial cycle (periglacial, glacial and boreal regimes) were conducted using the University of Toronto Glacial Systems Model (GSM). This model links with a wide range of geophysical, geological and geodetic data, such as sea level histories, ice margin positions and present day rates of rebound, to constrain the calculations and evaluate the degree of non-uniqueness in predicted ice-sheet histories and ground surface temperatures. One prediction of special interest for repository safety is the depth and extent of permafrost, and reasonable accuracy is found, for example, in the comparison of present day (and earlier time) predictions from GSM with field observations. GSM also predicts a permafrost "halo" will surround an advancing ice sheet, but the Earth's surface beneath the ice sheet could be at or close to the pressure melting point of the overlying ice. These studies demonstrate a basic understanding of glaciation effects over a timescale of approximately 10^5 years. Continuing work is aimed at understanding groundwater flow system evolution in response to glacial perturbations as part of an integrated multi-disciplinary framework ultimately aimed at supporting a repository Safety Case.

Regional and local groundwater flow systems on the Canadian Shield are strongly affected by fracture networks. The third host presentation (M. Srivastava) described recent work to create realistic 3-D fracture network models (FNMs) that are fully consistent with geoscience information typical of that available during surface based characterisation of a candidate repository site. Most of the detailed information would be on the location of surface lineaments from remote sensing and field observations. Other information would include data on regional stress fields, principles of geomechanics and structural geology, and relevant data from analogous sites. A procedure called Sequential Gaussian Simulation (SGS) uses a set geostatistical rules derived from direct field observation to develop probabilistic 3-dimensional fracture networks that honour all available geoscience information, including fracture location. In addition, SGS can readily incorporate new field data that may become available during site investigation, such as borehole and other subsurface studies. Verification of SGS, using detailed fracture mapping data from the Lägerdorf quarry is one means by which the applicability of the method has been tested. A primary benefit of the FNM methodology has been a strengthening of a more transparent connection between field data collection and synthesis through generating a constrained interpretation of fracture network(s) geometry that can be applied consistently in many site characterisation studies, ranging from modelling groundwater flow and transport to optimisation of repository geometry and orientation to minimise the likelihood of fracture intersection. Moreover, because the FNMs consist of a family of possible fracture networks, they can be used to explore geoscientific uncertainty and non-uniqueness, and the influence of these issues on confidence in repository safety. An example of such an application is included in the next presentation.

A safety case for a site on the Canadian Shield will require demonstrated understanding of the groundwater flow system and its potential evolution in the far future. The final presentation from the Deep Geological Repository Technology Program (J. Sykes and E. Sudicky) dealt with development of numerical modelling methods for simulation of groundwater flow and mass transport in crystalline settings. These methods provide a systematic framework to assemble multi-disciplinary geoscientific data sets into a comprehensive conceptual model of the geosphere. The conceptual model will be refined during the iterative site characterisation process that introduces an increasing level of detail in data from a wide group of geoscience disciplines. This presentation described three phases of study:

1. An illustrative numerical analysis of groundwater flow in a hypothetical Shield-like regional flow domain examined issues such as post-glacial evolution of the groundwater flow system, effects of complex surface topography, spatial rock mass distributions and the

occurrence of highly saline and anomalously elevated pressure heads described in sparsely fractured rock of the Canadian Shield.

2. A study at the sub-regional and repository scale focused on the integration and application of data management, numerical methods, visualisation and safety assessment. It used transient analyses for the simulation of flow (with coupled temperature, pressure and concentration) and the simulation of the impact of future glaciation. This second phase of study also examined issues such as the importance of large-scale fracture networks, explicitly embedding a fracture network model (or FNM described in the preceding OPG presentation).
3. The third phase of study involved comparison of two numerical models, FRAC3DVS and SWIFT-III, and investigations into fracture network uncertainties, the effect of salinity, spatially-correlated permeabilities and transient effects associated with glacial cycles (drawing from the glaciation studies in the second OPG presentation), including the influence of permafrost. The study of uncertainties used up to 100 different FNMs to estimate a probabilistic distribution of groundwater age, a performance measure of direct interest and value in exploring the case for safety and in optimising site selection. The glacial cycle study examined the depth of penetration of oxygenated glacial waters, a topic of particular interest for understanding the long-term performance of engineering barrier systems and radionuclide mobility. This third phase of study was also more firmly integrated with the MIRARCO Virtual Reality Technology Program, to illustrate and visualise the raw data and simulation results in a spatially and temporally consistent framework. This visualisation technology provides an enhanced understanding of the results from different geoscience disciplines and will create stronger linkages between these disciplines. More generally, the use of more representative and realistic conceptual models, coupled with visualisation technology, will enhance the ability of geoscientists to explain geoscientific concepts leading or supporting notions of far-field barrier performance and integrity and, hence, the repository Safety Case.

The last host presentation outlined some geoscience implications found in the CNSC draft Regulatory Guide G-320, “Assessing the Long Term Safety of Radioactive Waste Management” (P. Flavelle). The Guide recognises that geoscience information will play a major role in developing scenarios for use in safety assessments, which form the heart of a safety case in support of an application for a license from the CNSC. Safety assessments typically include a normal evolution scenario and may include scenarios of extreme events. The Guide also acknowledges that geoscience information might find additional applications in a safety case, such as to develop complementary safety indicators derived from the paleohistory of a disposal site. In addition, the Guide addresses issues such as transparency, clarity, quality control and quality assurance that apply not only to a licensing application but also to information collected prior to CNSC involvement (which may include site selection and characterisation activities). Specific suggestions for clear documentation include a description of how the geoscience data will be collected and used when preparing a site characterisation plan and provision of a “road map” in the safety case that describes where and how geoscience arguments contribute.

2.2 Key topics presentations

The central direction of AMIGO-2 was to examine how geoscientific arguments and evidence are linked in supporting a safety case. Authors of the key topic presentations were instructed to consider several specific questions in their talks. These questions, and a brief summary of the presentations, are provided below. The full papers are reproduced in Part B.

The first key topics presentation examined the potentials and limitations of geohistory to understand current features and conditions and possible future evolutions including the development of scenarios. The questions to be considered were as follows:

- Is the interpretation unique?
- Which uncertainties most affect the predictions?
- How do we deal with these uncertainties?
- How can present and past data be used to extrapolate future behaviour?
- How can geohistory support scenario development?

The presentation (M. Laaksoharju and P. Pitkänen) described recent work by SKB and Posiva (the Swedish and Finnish waste management companies) to understand the past and present evolution of groundwater in crystalline bedrock and overburden at sites bordering on the Baltic. The research indicates that the evolution of groundwater composition and distribution is influenced by flow, transport and rock-water interactions driven by past and present climate variations. Early stage work had not been comprehensive in considering inflows of different water types. In this study, brine, glacial, marine and meteoric waters undergo complex mixing at different depths during the different stages of a glacial cycle, further complicated by concurrent interactions with minerals contacted. Thus an explanation of current groundwater composition requires an integration of hydrochemistry and hydrogeology within a context of past geological events. The largest data uncertainties stem from "temporal disturbances from drilling" and natural variability; modelling or conceptual uncertainty includes the assumed composition of old water end members. Most of these uncertainties can be dealt with in a quantitative manner to give statistical confidence intervals on the modeled results. The benefits of this "geohistory" approach include prediction of future groundwater evolution and conclusions on potential groundwater residence time, two important topics for the safety case: two issues of clear importance in the safety case.

The second key topics presentation considered the transferability of data and information from other sites (repository sites, natural analogues or "generic" URLs) and considered the following questions:

- Which data and information did you transfer and for what purpose?
- Is there uncertainty associated with the transfer and how do you manage it?
- Is the transfer specific to a particular site or has it broader application?
- In a broader sense, what knowledge of concepts and processes is most amenable to transfer between sites?

The presentation (M. Mazurek, A. Gautschi, P. Marschall, W.R. Alexander, G. Vigneron, P. Lebon and J. Delay) drew largely from research on argillaceous rock in Switzerland and France. There are many reasons to transfer information among disposal sites, from underground rock laboratories and from natural analogues to disposal sites. For instance, data and understanding from other sites can fill gaps early in a developing programme, and confirm important observations and conclusions in a more mature programme. Information transfer also promotes the development of investigative tools and identification of model requirements, especially useful when dealing with complex issues of common concern. The presentation discussed different types of data and understanding and explored when they could be shared, and under what conditions. Numerous practical examples specific to argillaceous rocks underscored the value of transfer of information and provided support for an important observation: for argillaceous rocks, microscopic structure (largely determined by clay minerals present) provides a fundamental basis to permit valid transfers, and other relevant (but less important) factors include the degree of compaction, diagenetic cementation, make up of coarser-grained clastics and the in situ stress regime. More generally, the transfer of information must be justified using arguments that may differ for different types of host rocks. Successful arguments will be based on characterisation and understanding of relevant formation properties (such as microstructure, mineralogy, porosity, redox condition) and the physical states (such as stress and pore pressure). In principle (and for argillaceous systems with some extensions to other rock types), transfer is most straight-forward for parameters and features that do not depend on formation properties and physical states (such as thermodynamic and kinetic data). Transfer is also feasible for parameters and features that essentially only depend on a limited number of formation properties – in argillaceous rocks, these are most often mineralogy and porosity. Transfer is more difficult or impossible in cases when the sites have contrasting physical states.

The last two key topics presentations were concerned with the collection of geoscience data and information. The two presentations were somewhat unique in that they dealt with an operational disposal facility and they expounded upon the pragmatic experience of the implementer (R. Beauheim S. McKenna, D. Powers and R. Holt) and the regulator (R.T. Peake, C. Byrum and S. Ghose). The first presentation gave the implementer's view on the potentials and limits of the collection of geoscientific data and information for characterising the site. It examined the following questions:

- What types of data have been integrated?
- What uncertainties most affect site characterisation?
- How are these uncertainties addressed?

The facility described is the WIPP (Waste Isolation Pilot Plant) site in New Mexico, which was certified for disposal of transuranic and mixed waste in 1998. Site characterisation began over 30 years ago and to date has involved a large number of studies, including logging and testing of more than 100 boreholes, shaft and repository mapping, geochemical sampling, and hydraulic testing within, above and below the host formation. Integration of the large volume of resulting data has led to a robust model of the WIPP geology, but geoscience studies are continuing to resolve residual uncertainties and to improve predictive capabilities with regards to the cause and distribution of fractures in formations above and below the host formation. Much of the recent studies have been conducted on a particular stratum, the Culebra, which has been identified as the most likely groundwater transport pathway for radionuclides released via an inadvertent human intrusion scenario. Data from approximately 500 boreholes, outcrops and shaft exposures have been used to define stratigraphic and facies variations, leading to predictions of fracturing and transmissivity in the Culebra. Uncertainties remained in areas where information on the Culebra was lacking, and a new drilling and testing programme was initiated in 2003 to fill the more significant gaps in data. The study results have led to a probabilistic description of transmissivity fields in the Culebra which has then helped to bound the uncertainty in radionuclide travel times to the WIPP boundary. The study results have also identified where new wells might best be located to reduce uncertainties most effectively in future recertification activities.

The related (and final) key topics presentation was from the WIPP regulator (the US Environmental Protection Agency) and described the requirements for documentation of geoscientific data and understanding used to characterise a repository site (often called geosynthesis) and to support development of the safety case and its communication. It dealt with the following questions:

- How do you balance diverse input from various disciplines to synthesise lines of evidence?
- What regulatory guidance exists for structuring the documentation?

- What are the needs and mechanisms for interaction between regulators and implementers during the site characterisation?
- What processes exist to deal with issue resolution between implementer and regulator?
- How do you ensure that the documentation supports the needs of the scientific community reviewing the safety assessment?

Regulatory review of the WIPP site began almost 20 years after start-up of site characterisation activities. The objective of the review was to determine whether a licensing decision could be made, and required consideration of the technical merit, public concerns and legal issues. Balancing diverse input from a regulatory viewpoint led to the creation of fundamental questions that must be addressed by the implementer's documentation. Two introductory questions (is there enough information to make a determination and to what extent can the characteristics of the site provide a barrier to radionuclide migration) and subsidiary questions helped to balance information from diverse disciplines. Specific regulatory requirements were available and a "compliance application guidance" document provided further direction in check-list format. For example, confidence requires well-established quality assurance programmes that describe all elements surrounding the collection (e.g. procedures and source), processing (e.g. data reduction and analysis) and use (e.g. in performance assessment software) of data and other geoscience information. Confidence can be further enhanced through mechanisms that permit two-way interactions and resolution of issues between the implementers and regulators. Formal and informal interactions were involved and only occasionally did it become necessary to seek managerial intervention to resolve issues. An important thesis of this presentation concerned the essential need for confidence in the implementer's work:

> *"Confidence in repository site geoscientific data enhances the regulator's ability to make a credible and defensible certification (licensing) decision and to communicate the basis for the decision to the public. Lack of confidence in the data can lead to a lack of credibility about site suitability."*

Based on their practical experience, successful certification of the WIPP site came about because the regulators had provided a clear indication as to what documentation was required and the implementers produced high-quality documentation. The process was not always smooth, but it did lead to a certification that met technical review and legal challenges.

2.3 Plenary discussion

This discussion followed the host and plenary presentations. The suggested topics concerned the use of geohistory, transferability of data and information, collecting site characterisation data, and geoscience documentation requirements. For the most part, the discussion looked into differences and similarities in the roles and responsibilities of the national regulatory authorities.

- In Canada, the CNSC is responsible for licensing all nuclear-related facilities but their formal involvement starts only after an applicant applies for a license and submits the applicable fees. Informal reviews are carried out if time and resources allow. Ontario Power Generation desires closer involvement in future activities and may pre-pay licensing fees.
- In Sweden, the Swedish Nuclear Power Inspectorate (SKI) follows closely activities such as site investigation and modelling conducted by the Swedish Spent Fuel and Waste Management Company (SKB). There are review meetings twice a year, and include representatives from the Swedish Radiation Protection Institute (SSI) and international experts. These meetings have minutes that include a list of issues. An issue can only be

retired from the list when an acceptable response has been delivered. While there is no requirement on SKB to resolve these issues, it is clearly in their interests to do so.

- The situation in the U.S. is arguably more formal and involves the U.S. Department of Energy (US DOE) as implementer, and the Environmental Protection Agency (US EPA) and Nuclear Regulatory Commission (US NRC) as regulatory authorities. The US DOE is the proponent for both WIPP and the Yucca Mountain project. The US EPA regulates WIPP and the US NRC regulates the Yucca Mountain project. Meetings between representatives of the proponents and regulators are generally required to be public and all communications must be on the public record. The reason given for these requirements was the US EPA relied heavily on the contents of publicly available information for a legal defence of their regulatory decisions regarding WIPP.

- As noted in the final topics presentation, the US EPA was involved late in the site characterisation process for the WIPP site and adopted a "risk-informed" approach to make their review process more efficient and effective.

- The French safety authority established a "safety rule" in 1991 which included criteria for site selection. As in many other countries, these rules are expected to evolve as the waste management studies become more mature. For instance, the US EPA regulations are generic but more prescriptive requirements can be added to a license so that specific inadequacies are identified and corrected, and one specific example cited concerned requirements for quality assurance affecting documentation of data for the WIPP site.

- A comment that met with general agreement was "subjectivity lowers the product quality". This comment refers both to preparation and review of geoscience documentation. There must be solid scientific support underlying geoscience data and understanding, with concurrence from the entire team responsible for the work. Consequent review comments must also be prepared in a professional manner, and again require agreement from the entire review team.

3. SUMMARY OF THE WORKING GROUPS DISCUSSIONS

3.1 Working Group A: Geoscience indicators for safety

Working Group A continued deliberations started in AMIGO-1. Participants were asked to direct their energy toward the following questions:

- List different geoscientific arguments or indicators for safety (with motivation) for various host rocks and sites. Consider dividing the arguments into those that support isolation or retention and discuss their applicability for different time frames.
- What actual measurable field evidence supports these arguments/indicators?
- What kind of field evidence would go counter to these safety arguments?
- What key messages are the most promising in terms of scientific credibility to contribute to the safety case? Possibly examine the same message but in terms of potential ease of communication.

The discussions started with two presentations (reproduced in Part B): the first dealt with evidence for and implications of the existence of very old groundwater at Sellafield (Norris *et al.),* and the second described pertinent time frames needed to build a coherent hydrodynamic model of the Paris Basin (Violette *et al.*).

The Group's foremost achievement was the generation of a table that summarises the current status of geoscience arguments. The table (see Part B) defines five categories of safety functions:

1. groundwater flow predictability;
2. retention of potentially released radionuclides;
3. predictability of groundwater composition;
4. mechanical/geological predictability of the host formation; and
5. absence of resources in the host rock.

The tabulated discussion for each safety function includes an identification of the associated chains of arguments and reasoning, the relevant type of host rock or site, and consideration of the applicable time frames. Further discussion is concerned with field and other evidence that would tend to negate these arguments and comments on the key messages for use in a safety case. The Group also brought forward several simple and pragmatic conclusions:

- The most important geoscience argument is a clear understanding of the past geological history at the particular site. It should be consistent with a global understanding of geological evolution and have a broad consensus among independent experts.
- Most geoscience indicators for safety are based on a chain of arguments that together are stronger and more powerful than any individual argument.

- For the most part, the goal of geoscience investigations should be "reasonable" predictability. It should be recognised that the safety case could be made and defended if we can supply well-reasoned bounds on future evolution, as opposed to a detailed description.
- The same type of argument can generally be developed for different host rocks, although the strength of the argument and its time scale of validity might vary. The arguments are usually best suited to "simple" systems.

The Group also concluded that sharing experiences from different programmes is a crucial form of peer review and will lead to improved geoscience arguments.

3.2 Working Group B: Communication of geoscience safety arguments

Working Group B was directed to examine what modes (method, type of information, specific arguments) work and do not work for audiences such as colleagues and peers, authorities and regulators, political decision makers, the academic community, and members of the general public (adult and youth). They were to deal with the following issues:

- What are the actual experiences with respect to the stage of each programme?
- What is the place (for various audiences) of geoscientific arguments in relation to various other quantitative and qualitative topics like scenario and FEP assessment, simulated repository evolution for various scenarios, calculated dose or risk impacts, engineering tests of materials, etc., when presenting a safety case to different audiences and with respect to various stages of the repository programme?
- Would we be better off focusing messages to the public on time scales of a few hundred years or a few generations rather than on the much longer time scales considered in performance/safety assessments?
- How do you handle the fact that geoscience interpretations seldom are unique and often are open to various interpretations?
- How do you handle expert controversy on a specific topic?

The Group observed that communication experience, and the level of geoscience understanding, is very dependent on the stage of development of different national programmes. Geoscience information can be directed at various audiences, but different methods must be employed to be successful. Detailed information is best directed at experts in particular disciplines, but more general topics like scenario descriptions can be of interest to a broader range of audiences. With regard to time scales, the public and less technical audiences may be more interested in times affecting a few generations; however, it is likely that they will also need geoscience information that pertains to longer time scales. It may be more difficult to convey to the public the degree of confidence associated with time scales of the order of a million years. Controversial issues become more difficult in a public arena and can be resolved by early communication and by studies conducted by independent experts. Other suggestions and recommendations from Working Group B include the following:

- Different means of communication must be used, but the underlying information must be consistent and based on sound geoscience understanding. For instance, good illustrations are effective communication tools but they must be firmly based on the science and consistent with related illustrations and figures.
- Good illustrations take time, energy, and clear mental processes to produce.

- Communication should involve media people and geoscientists and appropriate training of both groups is recommended. For many (perhaps most) audiences, it may be more effective to improve the geoscientists' communication skills rather than to teach geoscience to a communication expert.
- The disposal development programme is a long process that will likely take many decades, from early conceptual studies to decommissioning and closure. Thus there is a need to reach young people, as they will be our decision-makers in the future.
- Communication between the implementers and their regulators should start early in the process and might be best served by informal reviews that help to identify and then resolve important issues.
- An effective way to deal with non-unique interpretations is to address each major possibility formally in the safety case.
- A management strategy to deal with public controversy involves preparation of a public report by an independent expert.

3.3 Working Group C: Realities of site investigation

Working Group C was concerned with first-hand practical experience related to limits imposed by the practicalities of site characterisation. It was to consider various host rocks and stages of the repository programme. The Group was asked to focus on the following expected outcomes and questions:

- List concrete examples of limitations on site investigations and their reasons, e.g. impossibly long time frames, high degree of heterogeneity, potential for impairing safety features of the host rock, etc. In addressing these issues, consider the relation between what you can measure and what you would like to describe.
- Can these limitations be handled by defensible uncertainty descriptions?
- What has been your experience in predicting properties/responses and then making comparisons with subsequent measurements? How much "after-fitting" was necessary? Did the exercise contribute to validation? What did it teach you about your abilities to characterise?
- What are the realities of transferability of data between sites? What can actually be transferred (data, conceptual models, evaluation procedures) and what could not?
- How have the experiences on possibilities and limitations influenced your investigation programme?
- How are the limits in what can be achieved factored into safety assessment and engineering?

The Group discussions started with two pertinent presentations (reproduced in Part B): one on the feasibility of parameter spatial extension and estimation of the uncertainty of permeability (Fedor and Szűcs), and another dealing with complex faulting structures and uncertainty in crystalline rock (*Geier*).

The Group examined in some detail limitations associated with the determination of K_d (distribution coefficient) data. The example centered on in-situ and lab testing, and the Group observed that *in situ* tests generally have more uncertain chemical conditions which reduces accuracy, and in-situ tests take longer to complete. The completion time can be an important limitation if time constraints are operative. Fortunately, it may be sufficient to determine that a K_d is larger than some minimum value but requires strong links to safety assessment. Another limitation concerns whether the data required are conservative or best estimate; conservative data require simplified models while best-estimate data use more complex models.

The effort needed to manage uncertainties depends on how far the results are from compliance limits. A conservative approach can be followed to bound uncertainty, but this could lead to inconsistency between data and models and a less comprehensive safety case. Site characterisation should avoid conservatism and make more use of realistic modelling. Unfortunately, modelling is not considered an efficient tool in site characterisation for reasons that include: the modelling effort lags behind data collection, the data samples are too sparse, and some properties of interest cannot be directly measured. Results from long-term experiments are important but adversely affected by degradation of sensors, the introduction of perturbations associated with the experiment, and cost.

The Group felt that multiple lines of reasoning (or a conservative approach) could compensate for characterisation limits, but there must be agreement between the implementer and regulator. Sensitivity analyses could play an important role in supporting or augmenting multiple lines of reasoning.

3.4 Working Group D: Assembling geoscience knowledge and arguments

Working Group D examined the assembly and integration of geoscientific knowledge and arguments based on actual experiences from the working group. The session started with a presentation (reproduced in Part B) on the assessment of uncertainty and confidence in the Site Descriptive Models (SDMs) being developed by SKB (Andersson *et al.*). The Group then proceeded to address the following questions:

- How do you manage integration between various geoscientific disciplines? How do you communicate this integration? (This issue is a continuation of the discussion from Working Group C in AMIGO-1 but should examine more recent practical experiences).
- In developing the site characterisation and evaluation programme, what experiences exist with feedback (e.g. conclusions drawn from sensitivity analyses, FEP-screening, etc.) from safety assessment and engineering? How is the exchange of information managed?
- How is geoscientific knowledge, including uncertainty, in “descriptive models” actually assembled and presented?
- How are geoscientific data and arguments actually used in safety assessment? What should be the balance in a safety case between geoscientific arguments and safety assessment calculations?
- How are the geoscientific data and arguments actually used in repository engineering (repository layout, design of underground excavations, etc.)?

The description of the SDM helped guide subsequent observations on two broad topics:

1. Managing integration. The Group noted that an integrated model is constructed by combining the models produced by different geological disciplines such as geochemistry and hydrogeology. An integrated model generally represents a best-estimate current description of the site plus uncertainties; it does not include a repository and conservatisms are left to the safety assessors.

Managing integration involves a great deal of communication and coordination within an iterative process, requiring processes to accept input from various technical experts and integration through multidisciplinary reviews and formal procedures for data management and acceptance. A common terminology for the variety of specialists involved is crucial for a successful integration. This "human-oriented" integration is followed by "code-orientated" integration, which has greater consistency if different disciplines use the same core model and database. A co-ordinating group with interdisciplinary skills is needed to direct the integration.

2. Handling uncertainty. Uncertainties exist in the raw "point" data, discipline-specific models and the integrated model. All uncertainties must be formally evaluated and documented, using processes such as responding to lists of focussed questions and discussion at interdisciplinary workshops. Depending on the nature of the uncertainty in question, the result might be alternative conceptual models, probability density functions or other qualitative or quantitative descriptions. Uncertainty might be constrained using multiple lines of evidence and studies of past evolution of the site. Other important factors include feedback from safety assessment and engineering and regulatory context or guidelines.

Working Group D had a final observation concerned with evolution in time of the site. The SDM represents the current description of the site and there is a need to deal with integration and uncertainty issues that may arise as the system evolves in the future. The Group observed that time evolution can be described using scenarios, which should be defined through an integrated, multidisciplinary process, based on common assumptions, to ensure self-consistency in the scenario descriptions.

4. PLANS FOR AN AMIGO GEOSCIENCE COMPENDIUM

On the last day of the workshop, a special presentation was made on plans for a unique outcome of the AMIGO workshops: the preparation of a geoscience compendium (Röhlig *et al.*). This product would be an AMIGO report that provides guidance and serves as a reference on how geoscience can strengthen a safety case. It will also serve to broaden awareness and knowledge, beyond geoscientists, as to our current understanding of the safety functions of the geosphere and our current confidence in that understanding. The idea for such a document was first discussed in the AMIGO Steering Group and a plan was approved by the IGSC in 2004.

Recent developments include the preparation of a questionnaire (with special thanks to volunteer testers, G. Bruno and C. Serres from IRSN, J-O. Selroos from SKB, and A. Gautschi, P. Zuidema and J. Schneider from Nagra) designed to capture information on generic and specific undertakings during geoscience investigations for a deep geological repository within sedimentary (clay, carbonate, evaporite) and crystalline settings. The desired information will be pertinent to long-term performance of radioactive waste repositories, with a timeframe extending to 10^6 years. The specific goals for the questionnaire are to:

- collect examples of geoscience lines-of-evidence that directly support or convey confidence in the performance of repositories in varied geologic settings;
- consider techniques used for effective communication of geoscientific reasoning and perspectives that support the safety case for a deep geological repository;
- identify methods and procedures that provide the geoscientific basis for the safety case, notably the geosynthesis or integration of multi-disciplinary geoscientific information and approaches that can constrain geosphere non-uniqueness and uncertainty; and
- explore methods related to planning and organising, to improve the manner in which geoscience information is collected and communicated.

The implementers who are responsible for developing a deep geological repository will likely have devised most of the geoscience arguments. However, to maximise its utility, the compendium should include viewpoints from the regulators whose background and understanding is unique. Regulatory comments might identify known examples that best satisfy national regulations, that are most useful in promoting public understanding, or that show promise but require further effort.

The questionnaire includes some sample geoscience arguments. One example is concerned with the safety function related to restricting contaminant transport, and explains how diffusive barriers can provide this function. The example then goes on to describe multiple lines of evidence that show the Opalinus Clay is a diffusive barrier. Although this example was taken from the recent Nagra safety case for Opalinus Clay, it is important to note that the safety function argument and the multiple lines of evidence can be readily adapted to other host rocks.

The NEA released the questionnaire in September 2005 (NEA, 2005). Potential respondents include national programmes for deep geological disposal, national regulatory agencies and even individual geoscientists. Approximately 14 organisations have confirmed their participation. The planned completion date for the questionnaires is October 2005. A draft compilation of the responses will be prepared by January 2006 and the first draft of the compendium is scheduled for June 2006.

5. CONCLUSIONS AND RECOMMENDATIONS

5.1 Observations and recommendations

Many enlightening and informative statements were made during the various meetings. Some noteworthy examples are collected below:

- In some programmes, “safety case” and “safety assessment” have been set apart to highlight an important distinction. Simply put, safety assessment refers to a specialised evaluation of the expected performance of a repository in relation to regulatory criteria, whereas safety case includes the safety assessment and all other information that may bear on understanding how a repository might function in the distant future. Geoscience is important to both: it provides a conceptual model (and data) describing the geosphere for use in a safety assessment and it can also provide much more information, such as evidence that supports the existence of a natural diffusive barrier or the effective isolation of a deep repository from external perturbations. Engineering information (on the engineered barriers) can also feed both the safety case and safety assessment.
- International geological disposal programmes share common issues such as the development of suitable field and laboratory tools for site investigation, the development of quantified descriptions (models) of the geosphere that include uncertainty and non-uniqueness and that integrate information from different disciplines, and the development of better documentation and communication tools.
- There are many geological and related disciplines of general interest, including climate change (e.g. glaciation); understanding movement of deep groundwater, subject to the effect of fractures, faults, saline gradients, diffusive barriers and more; paleohistory such as the geochemical evolution of deep groundwater, including the influence of mixing with meteoric water; and the development of conceptual and computer models that effectively integrate information from these disciplines. There are many challenges but the geoscience community is providing convincing evidence of their understanding, for example by using past glaciations to explain present day observations.
- All studies require thorough documentation that meets stringent requirements for transparency, clarity, quality control and quality assurance.
- The uniqueness issue can be very problematic. Generally, uncertainties can be reduced with more data and better understanding. However it may not be possible to eliminate outright all feasible options and it would then be prudent to examine systematically such options in the safety case. Often simple scoping studies might suffice to show that many options need not be carried forward because, for example, they do not lead to or imply any significant impact in the repository evolution or performance.
- An explanation of current groundwater composition requires an integration of hydrochemistry and hydrogeology within a context of past geological events. It must also deal with uncertainties, notably those associated with system heterogeneity and the initial

and boundary conditions. The benefits of this “geohistory” approach include prediction of future groundwater evolution and conclusions on potential groundwater residence time.

- Transferability of data and information from other sites, laboratories and analogs is a valuable means to fill gaps in data and understanding (especially at early states), to confirm important observations and conclusions, and to promote development of investigative tools and identification of model requirements.
- The transfer of data should not be ad hoc but follow a predefined logical structure. Uncertainties arising from the transfer of data and information are best minimised if there exists a fundamental basis that allows valid transfers. That is, the transfer of data and information must be justified using basic scientific arguments; these arguments may differ for different types of host rocks. In the case of argillaceous rocks, transfer is most transparent for parameters and features that do not depend on formation properties and physical states; more difficult but still feasible for parameters and features that depend on a limited number of formation properties (mineralogy and porosity); and difficult to impossible when physical states are dissimilar. Well-reasoned scientific arguments can likely be developed for other sedimentary rocks and for crystalline rocks.
- Clearly we can expect uncertainties to decrease as more information becomes available. That is, a maturing programme will lead to more confidence in the description of the geosphere (or the conceptual model), potential scenarios and data for particular parameters. In part, this result will come about because we can focus resources on issues for which residual uncertainties are most significant. In addition, our improved understanding will permit better identification as to what uncertainties are most significant, and better prediction of how to resolve these uncertainties.
- Effective interactions between regulators and implementers are essential to facilitate the review processes and to build confidence in the predicted outcomes of the safety assessment. The regulator should establish a clear and comprehensive set of regulations, and provide guidance and direction on critical issues. The implementer should openly communicate research results and fully document the safety case and supporting documents. This documentation must include elements of quality assurance, describing (for example) the process and results that involve collection, processing and application of geoscience data in the safety assessment and the safety case.
- There is a role for both formal (public) and two-way interactions between the regulators and implementers. A mechanism to resolve issues should be prescribed.
- Confidence in repository site geoscientific data enhances the regulator’s ability to make a credible and defensible licensing decision and to communicate the basis for the decision to the public.
- There are important differences and similarities in how the national regulatory authorities fulfil their responsibilities.
- There are numerous similarities in the geoscience programmes for nuclear waste disposal and for geosequestration of CO_2. There is an opportunity for cross-pollination of information and tools, and certainly for knowledgeable critical review.
- WG A: A useful geoscience focus for demonstrating safety is on five categories of safety functions and the associated chains of argument and reasoning: (i) groundwater flow predictability, (ii) retention of potentially released radionuclides, (iii) predictability of groundwater composition, (iv) mechanical and geological predictability of the host formation, and (v) absence of resources in the host rock. These categories influence the

three main roles of the geosphere, which are (1) to provide isolation from the human environment, (2) to prevent, delay and attenuate radionuclide release and (3) to provide a stable chemical and physical environment that is insulated against external perturbations. The most important geoscience argument is a clear understanding of the past geological history at the particular site; this should be consistent with a global understanding of geological evolution and have a broad consensus among independent experts.

- WG B: A major goal of geoscience studies is their full integration with the safety case; for instance, presenting geoscience results is not a goal in itself, but presenting geoscience results and the way they affect safety is indispensable.
- WG C: The intended use of data affects its acceptable uncertainty. For example, it may be sufficient to demonstrate that a measured K_d is larger than some minimum threshold value.
- WG D: Uncertainty might be effectively reduced or constrained using arguments that are based on multiple lines of evidence and studies of past evolution of the site. These outcomes will require multidisciplinary discussions and review.

5.2 Recommendations concerning AMIGO-3

Members of the AMIGO Steering Group and the AMIGO-2 Scientific Programme Committee made several recommendations to be considered further during the planning for AMIGO-3, the final workshop of the AMIGO series. These recommendations include the following:

- The structure of the AMIGO-2 workshop, slightly modified from AMIGO-1, was effective in allowing more time for discussion within the working groups. The in-depth discussions of the host group and the key topics presentations were also well received. Another noteworthy change was to the lists of questions used to guide the key topics and keynote presentations, and the discussion of the working groups. These questions were somewhat more focused than was the case in AMIGO-1 and directed the deliberations to key issues. The structure for AMIGO-3 might also evolve, depending on its needs, but the structure of AMIGO-2 is a recommended starting point.
- A good focus for AMIGO-3 would be on applications of geoscience arguments in the safety case. It should deal with links to the safety assessment, the qualitative and quantitative use of geoscientific information and feedback to and from the safety assessors and the geoscientists. A main result from AMIGO-3 would be an indication of whether geoscience arguments are (or will be) effectively addressed in safety reports. This implies more input from safety assessors than in the previous workshops.
- AMIGO-3 will conclude the AMIGO workshops. It is possible that AMIGO-3 and the planned AMIGO compendium, together with the outcome of other IGSC activities like the EBS initiative, would give reasons to update NEA documentation concerning safety assessments and the safety case.
- A potential key topic that might be explored in AMIGO-3 concerns a broader feedback subject that connects the safety case, fundamental geoscience R&D, development of effective engineered barriers and site characterisation studies. Issues to consider include geoscience information to be transferred (including data usage, upscaling and simplification issues), justification of processes or effects to be considered or ignored in different scenarios, conservatism *versus* realism and quantification (or other treatment) of all sources of uncertainty.

- Another key topic might examine the development of new geoscience tools and perhaps comment on whether time is the only solution to bridge the gap between modelling and characterisation.

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PART A

REPORTS OF THE WORKING GROUPS

Working Group A: Geoscientific Indicators for Safety

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Working Group A was continuation of Working Group B of AMIGO-1, but participants explored more deeply the issues surrounding geoscientific indicators for safety. The following outcomes were expected.

- List different geoscientific arguments or indicators for safety (with motivation) for various host rocks and sites. Consider dividing the arguments into those that support isolation or retention and discuss their applicability for different time frames.
- What actual measurable field evidence supports these arguments/indicators?
- What kind of field evidence would go counter to these safety arguments?
- What key messages are the most promising in terms of scientific credibility to contribute to the safety case? Possibly examine the same message but in terms of potential ease of communication.

The session started with the following two introductory presentations:

1. Use of Geoscientific Arguments in the Nirex Phased Geological Repository Concept: Illustrative Desk Study by S. Norris, B. Breen, and J.L. Knight (UK Nirex Ltd).

2. Past Geologic, Climatic and Geomorphologic Forcing Influence on Present-day Hydrodynamics, a Key to Understanding Future Evolution: Example of the Paris Basin, France by S. Violette, A. Jost, and J. Gonçalvès (UMR.7619-Sisyphe, UMPC, France), and the “Paris basin modelling” team.

Following the presentations, in discussion the Working Group listed:

- Safety Functions where geoscientific support is needed;
- Commonly used chains of argument for supporting these safety functions;
- Whether the applicability of the arguments are host rock or site specific and how they apply for different time frames;

- Field evidence or other issues that would go counter to the safety arguments;
- Key messages most promising in terms of scientific credibility to contribute to the safety case.

The findings are documented in Table 1.

Overall it was concluded by the Working Group that:

- The most important argument is to present a clear understanding of past geological evolution at the particular site, consistent with the global understanding of geological evolution. Efforts should be made to achieve a broad consensus on this from many independent experts.
- The supporting arguments are seldom based on a single piece of evidence. It is the chain of arguments rather than individual arguments that is important.
- We are primarily interested in "reasonable" predictability of the geological system. We recognise that most geological systems evolve with time, but all details of this are not needed for demonstrating safety. However, there is a need to find well-reasoned bounds for the future evolution.
- Generally, the same type of arguments can be applied for different rock types. The strength of arguments and the time scale of validity, however, vary between host rocks and types. The arguments work better in "simple" systems.
- Sharing experiences between different programmes is crucial in assessing strengths and weaknesses in "own" arguments

Table 1 **Safety functions, supporting arguments, challenges and key messages**

Safety function	Chain of arguments, with motivation	Host rock or site-specific and applicability different time frames	Field evidence or other issues that would go counter to the safety arguments	Key messages most promising in terms of scientific credibility to contribute to the safety case
Arguments for groundwater flow predictability.	Evidence in the past showing an understandable evolution of the groundwater flow. Important arguments include: • Age of groundwater (hydrogeochemistry, isotopes, noble gases). • Composition in equilibrium with host rock. Is the stability easily explainable by groundwater flow modelling – what is the reason for stability (stable because of salinity gradient or low hydraulic conductivity). Analogue information/reasoning.	Most type arguments can be applied to different rock types, with some exception for salt? The strength of arguments and the time scale of validity varies between host rocks (and sites). Example motivation for salt: Salt itself is impervious. Predictability of flow in the overburden depends primarily on the permeability data, characterisation of brine inclusions in the salt, existence of the salt formation. Example motivation for more permeable systems: The combination of geochemical arguments of age/origin and consistency with groundwater flow modelling. (Strengths of argument depend on time frame considered and is also host rock specific, e.g. impact of glaciation in 10ka time frame, assessment of argillaceous systems in 200Ma time frame).	Indications of young water (including ^{3}H, ^{137}Cs) at repository depth, (would at least make the hydrodynamic analysis more complex and harder to define). Uncertainties in chemical analyses modelling (e.g. noble gas). If palaeohydrogeology is complex/very uncertain (like glaciation) there may be a limit to how far hydrodynamic modelling can be supported (problems in defining good initial/boundary conditions). Complex permeable structure media (strongly heterogeneous), makes hydrodynamic analyses more open-ended. Other counter arguments: Impact of the repository itself, investigation boreholes (on the permeable features), depends also on the repository operation time and layout. Impact from the waste (thermal buoyancy, gas generation.	The arguments work better when they result in a relatively simple overall description of the findings, e.g. salt would have dissolved if there were too much flow. (This is even more true in communicating with the public). Note that, for repositories in salt formations, sometimes different chains of argument may be appropriate. This recognises that salt provides (at least for the repository post-closure period in the reference case “normal evolution” scenario) complete containment of the waste.

Table 2 **Safety functions, supporting arguments, challenges and key messages** (cont'd)

Safety function	Chain of arguments, with motivation	Host rock or site-specific and applicability different time frames	Field evidence or other issues that would go counter to the safety arguments	Key messages most promising in terms of scientific credibility to contribute to the safety case
Retention of potentially released radionuclides	Low measured permeability. Flow model consistent with geological structure model (but uncertainties in geological structure model, and needs for additional assumptions). Age of groundwater (hydrogeochemistry, isotopes, noble gases) – however alter-native interpretations and will this exclude possibilities of fast pathways? Measured diffusion profile (e.g. Opalinus Clay etc. studies). Ensure that tests are made for the important properties and formations (c.f. testing cap rock permeability for gas storage). Pieces of evidence (flow field, lab-diffusion tests, sorption data, etc), but how to prove the upscaling?	Measured diffusion profiles: used as arguments for allowing discarding advection as transport mechanism. Retention arguments are especially needed for the long time frames. Modelling will indicate in which formations the retention arguments are most needed. In host rock with potential for diffusion dominated transport (argillaceous, shale etc.) field evidence for diffusion profiles appear to provide very strong arguments. In particular, diffusion profiles across faults – demonstrating that the fault itself would not be a major pathway. Sorption properties of the host rock material itself (clay minerals, rock minerals), determined in laboratory – combined with confirmatory in-situ measurements.	Existence of diffusion profiles may be due to other effects such as ongoing transient effects, poor understanding of the hydraulic driving forces (i.e. is profile the result of advection). Therefore diffusion profile evidence need to be combined with palaeohydro-geology modelling/assessment to ensure that currently measured situation is consistent with perceived evolution. Mechanistic understanding of retention processes is still under development (scientific arguments) – also implies uncertainties under which time frames sorption would exist and whether it is reversible or not. When arguments for retention are based on upscaling there will always be an uncertainty if it was done correctly (under-lying conceptual model) and how retention will be affected by future changes in flow boundary conditions and geochemical environment.	Retention is a naturally occurring phenomenon and can be demonstrated that it occurs naturally. Case for retention is easier in tight and homogeneous systems. (Potential for strong evidence of retention). Content of clay minerals strong argument for retention. Consistent evidence of matrix porosity.

Table 3 **Safety functions, supporting arguments, challenges and key messages** (cont'd)

Safety function	Chain of arguments, with motivation	Host rock or site-specific and applicability different time frames	Field evidence or other issues that would go counter to the safety arguments	Key messages most promising in terms of scientific credibility to contribute to the safety case
	In situ (tracer test), but can be serious restrictions in testable scales and upscaling for conclusions to be drawn, depends on host rock)/ Evaluation of natural tracers (evolution of salinity, ^{3}H, other isotopes,)	In crystalline systems, existence of high flow paths means that there is a need to show evidence of matrix diffusion along migration paths. (Done by lab-scale diffusivity tests, combined with *in situ* porosity measurements (electrical conductivity).		
	Tightness of formation indicated by existence of petroleum resources (for some clay and salt sites). Host rock without permeability (rock salt). Natural analogues demonstrating the long term existence of retention in general and that this also applies to radionuclides.	In crystalline systems there is also a need to show sufficient understanding of distribution of flow paths ("flow wetted surface"). Potential for retention in crystalline media by sorption in the fracture infill would depend on ability to determine distribution/existence of clay material in the infill. In salt system, the salt itself is impervious. However, all above arguments apply for the rock surrounding the salt formation.	Artificial in-situ tracer tests sometimes difficult to assess meaningfully – retention in appropriate rock often so strong that breakthrough would take too much time, i.e. limited to small test scales – hard to do in surface based field environment. Tests result could be hard to evaluate due to impact of competing transient processes. Would work best in "simple systems" (c.f. Mol site tracer test). Evaluation of natural tracer test important complement to upscaling. However, uncertainty in initial and boundary conditions may be affected by migration properties in "irrelevant" parts of the formation. Natural analogues – good for demonstrating existence of retention and for conceptual models, but always a question about transferability. Impact of the repository itself – creating additional flow paths (see above), changes of chemistry, production of colloids, *et al.*	

Table 4 **Safety functions, supporting arguments, challenges and key messages** (cont'd)

Safety function	Chain of arguments, with motivation	Host rock or site-specific and applicability different time frames	Field evidence or other issues that would go counter to the safety arguments	Key messages most promising in terms of scientific credibility to contribute to the safety case
Predictability of groundwater composition	Arguments for the hydraulic predictability (see above). Also the individual arguments used for showing under-standing of groundwater flow evolution. Understanding redox processes (absence of dissolved oxygen). Total dissolved solids, oxygen isotope analysis, hydrogen isotope analysis, and noble gas recharge temperature provide consistent under-standing of origin of water (e.g. sea, meteoric), and tempe-rature at time of recharge. Dissolved helium-4 content, chlorine isotope analysis, e.g. ^{81}Kr content, ^{129}I content, ^{234}U content provide groundwater age compatible with understanding of ground-water age and temperature at recharge. Bromide/chorine ratio in groundwaters (indicative of origins of salinity) can be readily understood in terms of observed geology; in agreement with content and stable sulphur isotope ratio of groundwater.	Most type arguments can be applied to different rock types, with some exception for salt? The strength of arguments and the time scale of validity varies between host rocks (and sites). Identification of discrete origin of groundwater composition more problematic in some host rock than others; with increa-sing time, greater probability that groundwater is a complex mixture of waters with no discrete origin. Groundwater age dating techniques based on radio-nuclide half-life analyses limited to groundwater younger than a small number (<10?) of half-lives of the radionuclide chosen.	Indications of oxygenated water at repository depth. Indications of "young" groundwater at repository depth. Impact of the repository itself, e.g., introduction of aerobic conditions at depth in rock adjacent to the repository, investigation boreholes (drawdown/upconing of "detrimental" waters). Gross inconsistency between understanding of groundwater evolution on basis of site investigation and laboratory analysis, and the results from hydrodynamic modelling – would fail to build confidence in understanding of behaviour of the site.	Develop a "storyboard" for the evolution of groundwaters at site that is consistent with the known geological evolution of the site (regional scale and at more local scales), and consistent with known palaeo-climatic under-standing. On this basis, pre-dictions for groundwater compositions in the region under investigation can be made, and tested by sub-sequent e.g. drilling analysis as part of confidence building. A degree of consistency between geochemical ages of the groundwater (from a site investigation programme) and groundwater travel times calculated by hydrodynamic modelling gives greater credibility to 'forward' modelling, and estimations of the future performance of a repository,

Table 5 **Safety functions, supporting arguments, challenges and key messages** (cont'd)

Safety function	Chain of arguments, with motivation	Host rock or site-specific and applicability different time frames	Field evidence or other issues that would go counter to the safety arguments	Key messages most promising in terms of scientific credibility to contribute to the safety case
	Absence of younger ground-waters at depth of interest. Analysis of secondary mineralisation in presents understanding of the palaeohydrogeology of the site that is consistent with other ground-water analyses. "Storyboard" for evolution of groundwaters at site is consistent with the known geological evolution of the site (regional scale and at more local scales), and consistent with known palaeo-climatic understanding. Hydrodynamic modelling of the region provides an understanding of forward and backward modelled pathlines, and related travel times for a 'particle' of groundwater, that are consistent with the hydro-chemical understanding of the age and history of the groundwater at the site.			

Table 6 **Safety functions, supporting arguments, challenges and key messages** (cont'd)

Safety function	Chain of arguments, with motivation	Host rock or site-specific and applicability different time frames	Field evidence or other issues that would go counter to the safety arguments	Key messages most promising in terms of scientific credibility to contribute to the safety case
Mechanical/geological predict-tability of the repository formation such that the integrity of the rock structure would not be impaired Determines the future conditions of the repository site. Requires sufficient predict-tability of future natural events (earthquake, fault activity, igneous activity, uplift, glaciation, thermal evolution etc.)	Geological understanding of the deformation history – when, why and how faults are moving, geological description of the past, understanding the tectonic regime, dating of lithology. Understanding of the mechanisms and the relationships in plate tectonics. Assessment of long-term stability of plate system by geophysical experts. If stable tectonic regime it is acceptable to extrapolate currently measured changes (e.g. uplift) into the future. Historical records of seismicity. Evidences of impacts of seismic events from other underground excavation (natural analogues). Geological characterisation of the site exploring evidences of past mechanical impacts (age of faulting, etc) – important argument for stating that future movement would only occur along existing faults. Large scale mechanical modelling of the impact of ice-loading, connected erosion.	The strength of the arguments varies between tectonic conditions. Not so much rock type dependent. However, dating of faulting becomes more uncertain when the sedimentary rock cover has been eroded. Need to avoid tectonically active area would depend on the tectonic setting. Need to consider impact of glaciation would depend on latitude and time frame for the assessment (or rather the historical evidence of past glaciations). However, there are glaciation impacts (hydrogeological) also outside the regions of ice cover.	There are limitations to predictability of future events – repository systems need to be shown robust against a variety of events – and a wide range of the specific conditions implied by these events. This is an important argument for deep geological disposal!! For example: Plate tectonics not fully understood. Mechanisms of climate change not fully understood. Uncertain human impact on glacial cycle evolution.	Important to present a clear understanding of past geological evolution at the particular site – and that this is consistent with the global understanding of geological evolution. (Strive for consensus from many independent experts). Underground is more mechanically stable (and would not be affected by erosion etc.) than the surface. Easier to demonstrate reasonable predictability in simple and currently "quiet" geological environment, but this is also a matter of scale (there can be stable domains also in a tectonically active region).

Table 7 **Safety functions, supporting arguments, challenges and key messages** (cont'd)

Safety function	Chain of arguments, with motivation	Host rock or site-specific and applicability different time frames	Field evidence or other issues that would go counter to the safety arguments	Key messages most promising in terms of scientific credibility to contribute to the safety case
	Is suggested repository depth sufficient in relation to uncertainty in erosion? Would existence of host rock depend on stability of surrounding formation (salt dome? overload formation need to preserve good properties of bedded clay formations). Predictability of seismic events. Rock mechanics data evaluation and rock mechanics. Analogue information and reasoning. Assessment of quaternary geology evidences of glaciation. Thermal profiles in boreholes Climatic (including glaciation) modelling – conditioned by observations on current system.			

Table 8 **Safety functions, supporting arguments, challenges and key messages** (cont'd)

Safety function	Chain of arguments, with motivation	Host rock or site-specific and applicability different time frames	Field evidence or other issues that would go counter to the safety arguments	Key messages most promising in terms of scientific credibility to contribute to the safety case
Absence of resources (mineral, water, oil, etc) – or other uses of the host rock	Common host rock type, preferably also present at out-crop in the vicinity of the repository - limits risk of being of interest in the future, and even if rock were to become an economic resource in the future, accessing it from the outcrop would be undertaken in preference to mining for it (& possibly inadvertently disrupting the repository). Simple/predictable geology. Let mining exploration company explore "mining" potential. The location of the facility at sufficient depth to reduce the probability of human disturbance (drilling frequency decreases with depth of rock penetrated).	Period of institutional control would mitigate early inadvertent intrusion. After institutional control period has lapsed, intrusion could, in theory, occur at any time(s) during the assessment time frame. From analysis of borehole drilling – target rock formation data in geological archives, a clear relationship is shown to exist between rock type and drilling frequency. Typically a sedimentary succession, due to associations with economic resources such as oil, gas, coal & water, is drilled into more frequently than a hard rock succession (which typically is less economically attractive). Also, investigating the potential of a sedimentary basin for CO_2 storage, or for geothermal resources, might motivate human intrusion.	When excavating a repository following surface-based investigations, a previously-unknown, economically significant geological resource is discovered. A site that is ideal today to host a repository facility might be considered in the future to host another waste management facility. If knowledge of the earlier repository was lost, inadvertent intrusion could result. Reliance being placed on persistence of institutional control in the shorter term following repository closure, and archives in the longer term – there is only very limited precedence for knowledge being passed to distant future generations in a form that is readily understood (both in terms of the context of the message being imparted, and the language being used).	Emphasise the safety function of deep geological waste management in reducing the likelihood of future inadvertent human intrusion. Details the main actions that could be taken to reduce the probability of future inadvertent human intrusion into a deep geological repository. Demonstrate that frequencies and doses have been reduced, as far as is practicable, through appropriate design and siting decisions and actions to preserve knowledge of the facility. Demonstrate that the location of the facility is at sufficient depth to reduce the probability of human disturbance. Evaluate the various actions that may prevent or mitigate the effects of a future human intrusion.

Table 9 **Safety functions, supporting arguments, challenges and key messages** (cont'd)

Safety function	Chain of arguments, with motivation	Host rock or site-specific and applicability different time frames	Field evidence or other issues that would go counter to the safety arguments	Key messages most promising in terms of scientific credibility to contribute to the safety case
	The use of site markers and archives to increase the probability that information about the site is retained for as long as possible. Use of repository materials that, when extracted from drilling operations, would be clearly distinguishable as different from the host rock (easily identifiiable as anthropogenic in origin?).	Note that, when considering the likelihood of human intrusion into a particular host rock, it is not just the economic potential of the host rock itself that needs to be taken into account: the host rock might be subjected to intrusion as a result of investigative drilling targeted on an economic resource at greater depth. The strength of argument varies between geological settings. The probability of inadvertent human intrusion into a repository located in a clay or evaporitic rock, from 'blind' hydrocarbon prospecting, is therefore likely to be higher than a inadvertent human intrusion into a repository situated in a rock of minimal economic potential (although this assumes as a basis loss of knowledge of the repository or the results of previous drilling into the host rock).	Common approach in human intrusion pathway is to assume current day technology. Future technologies might make accessing rock at repository depths much more routine, cheap and practical – this could redefine what is considered an economic resource, possibly negating the appropriateness of the choice of host rock. Repository produces geophysical or geochemical signature that encourages a future population, ignorant of the purpose of the repository, to intrude into it. Repository access tunnels and shafts, albeit backfilled with rock originally excavated during repository construction, might also attract interest due to having different properties (e.g. appearance, hydrology) from surrounding, unexcavated rock.	

Working Group B: Communication of Geoscientific Safety Arguments

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1. Main objective

Working Group B addressed the communication of geoscientific safety arguments through a discussion of practical experience as it related to the methods, types of information and specific arguments found to best communicate geoscientific concepts and notions of safety with broad audiences including, colleagues, authorities and regulators, political decision makers, academics, and the general public.

2. Main questions

The following questions were suggested by the programme committee of the AMIGO-2 workshop for discussion by Working Group B with respect to the communication of geoscientific information and safety arguments:

- What is the place of geoscientific arguments in relation to quantitative and qualitative topics like scenario and FEPs (features, events, processes) assessment, simulated repository evolution, calculated dose or risk impacts, engineering tests of materials, etc., when presenting a safety case to different audiences and with respect to the various stages of the repository programme? (see section 3).
- Would we be better off focusing messages to the public on time scales of a few hundred years or a few generations? (see section 4).
- How do you handle the fact that geoscience interpretations seldom are unique and data often are open to various interpretations? (see section 5).
- How do you handle expert controversy on a specific topic? (see section 6).

3. Variability of audiences – variability of communication methods

Participants recognised the diversity of the audiences to which geoscience information and concepts must be communicated. This variability requires the development of various methods to communicate, each method being tailored to the nature of the audience and the purpose of the information exchange. For each type of audience, the group provided suggestions for workable methods.

- Audience 1 – **Colleagues and peers**. National organisations should combine general, “complete” and site-specific integrated multi-disciplinary geoscientific descriptive model(s) of the site when developing a basis to explain/support the Safety Case to colleagues and peers. Establishing regular multidisciplinary meetings within the organisation has been found to be an effective means to share common views on geoscience, build confidence in the site understanding/arguments, and to reveal and manage inherent geologic uncertainties.
- Audience 2 – **Authorities and regulators**. Regulators are technical experts and “peers”. The supporting documentation when communicating to regulators should include a collection of geoscientific arguments in “Geosphere process/Geosynthesis reports” or correspondence. The purpose is to document the scientific understanding of processes to a level required for an adequate treatment in the safety case (e.g. as based on science, underground research laboratory results, surface laboratory experiments, natural analogues, etc.). Regular meetings within a constructive format and record of issues/agreements are also encouraged to build confidence within the stepwise decision making process. This communication should be initiated at an early stage.
- Audience 3 – **Politicians/decision makers**. These stakeholders need executive summaries with good illustrations and visual results in order to best understand the role of geoscience in the overall repository system with respect to national context and the site-specific safety case. The importance of technical visits by advisory groups or politicians to the waste management programmes of their own or other countries can not be underestimated as a means to develop understanding of waste management concepts and issues.
- Audience 4 – **Academic/scientific community**. This community requires clear and detailed technical/scientific reports documenting, among other factors, the evolutionary geoscience processes examined, spatial and temporal data sets, and the derivation of conceptual and predictive numerical models for repository adaptation, design and assessment. The publication of such project specific information in conferences and peer reviewed scientific journals by waste management organisations and their supporting research bodies is considered an effective method to obtain peer recognition and acceptance or validation of data interpretation and conclusions.
- Audience 5 – **General public (adult and youth)**. The Group acknowledged that this audience expects good illustrations that could be part of adequate and regular bulletins and/or reports (e.g. NAGRA bulletin). Methods found to aid confidence building with the general public include organised visits to research establishments, the creation of Information Centres and regular forums for open discussion e.g. public visits to nuclear waste transport ship in Sweden; public discussions in train stations in Switzerland.
- Audience 6 – **Environmental groups (with appointed experts)**. Some stakeholders may be quite sophisticated technically and have well-developed views (even specifically on geoscience issues) but nevertheless can also be difficult to convince through scientific/technical arguments. The group did not reach consensus on methods to deal with such groups other than to foster and maintain scientific credibility throughout the geoscientific work programme.

Beside the stepwise development of a comprehensive conceptual site descriptive model(s) as a basis for Performance Assessment (PA) and Repository Design, geoscientific arguments play an important and clear role in supporting the Safety Case. We need to develop different and adequate approaches/explanations according to the purpose of the communication and the type of audience. Communication is a long on-going process that lasts years during which decision making typically follows a step by step approach. Ideally, a dialogue on geoscientific safety arguments should be initiated at early stages, particularly with regulators, as this is a means to help build confidence in a Safety Case. Publication in international scientific journals should be a goal in attempting to reach the academic/scientific community and thus ensuring that the use and interpretation of geoscience information are transparent; are aligned with geoscience principles across fields; and take account of the most recent progress in research and academia.

There is no "universal" geoscience report to address all geoscience communication requirements as there are different levels of reporting of geoscience; presentation of the results will depend on the target audience.

The group recommended that training geoscientists in media relations may be more effective (and efficient) for meeting and communicating with the public instead of training media-relations persons in geosciences. Good, meaningful, and quality-based illustrations are considered as valuable tools appropriate to target audiences but they take time to be produced. The importance of site visits for political decision makers and the public was raised and should not be underestimated. Visits abroad to similarly proposed repository concepts and/or research facilities could be envisaged for organisations with no site.

4. Focusing messages to the public on timescales of a few hundred years or a few generations

The Group acknowledged that geologic timescales relevant to the demonstration of repository safety are considered a difficult issue to communicate within public forums. It has been the experience that the public is primarily concerned by short-term (several generations) issues as they relate to influence(s) on groundwater resources. It is possible in this regard that site-specific geoscience understanding, in addition to Safety Assessment, can provide intuitive and illustrative evidence to support explanations of 'non-release' during the short-term. Participants acknowledged the increased uncertainty associated with predictive assessment leading out to timeframes of 1 million years and the difficulties associated with instilling confidence in such assessments. They acknowledged that the public is sceptical towards such precedent setting predictions. One suggestion was to split the timescales in successive time scales and provide an assessment for each phase.

5. How do you handle the fact that geoscience interpretations seldom are unique and data often are open to various interpretations?

Building confidence in geoscience interpretation requires the adaptation and use of alternative hypotheses/conceptual models to illustrate reasons for differences and also the consequences of equally plausible explanations. A particularly useful technique in this regard has been the development of independent interpretations of the site data to re-affirm site understanding. It is suggested that during the interpretative process decisions should be traced at each step in the site characterisation programme.

Multiple lines of evidence could also be a way to argue a preferred model and/or interpretation. Geoscientific arguments could be used for non-technical audiences such as diffusion profiles of environmental tracer or natural analogues such as the preservation of wood.

6. How do you handle expert controversy on a specific topic?

Expert controversy means disagreement involving diverse opinions. Professional differences of opinion are not so important as far as they do not become publicly controversial. It is more difficult to manage when they are aired in public. Many differences can be mitigated or resolved with topical workshops with invited specialists as many controversies are the result of misunderstandings.

The group conceded that, in general, avoiding controversy by early communication (in particular with the regulator) is the most appropriate method to handle difference of expert opinion. Clear documentation of how data are interpreted, and having a transparent rationale for choosing one interpretation over another, can be useful in this regard. Additionally, the handling depends on the level of controversy – is it internal or external debate – and also on the significance of the issue in question with regard to safety. Internal and non-public issues are in principle easier to solve. However, with regards to external/public issues, participants suggested that disagreements may be arbitrated through work done by an independent specialist.

7. Conclusions and suggestions

- Illustrations are important tools but they must be based on sound and robust geoscientific knowledge. Illustrations also need consistency in presentations, in particular consistency between figures and related data tables are necessary. Good illustrations take time to produce.
- It is important to create a systematic framework for the interaction of multi-disciplinary groups who will integrate the geoscience information/data. This can be crucial in fostering a clear understanding of the Safety Case, geoscience data needs and how geoscience arguments can best be positioned to lend support.
- Long-term radioactive waste management and, in particular, repository concept implementation involves a long multi-year process. There is a need to reach young people as they may be our decision makers in the next generation.
- Training the scientist to communicate is a method to better promote geosciences to non-specialist audiences. Organising university seminars is, for instance, a good platform for training.
- The implementing organisation should be prepared for many audiences and with the expectation that initiating communication early in the process is preferred.
- “Radwaste words” are sometimes difficult to understand. This is considered a weak point when communicating geoscience to both experts and public. It is recommended that specialist nomenclature be avoided to the extent possible. There is a need to simplify vocabulary, while at the same time taking care to use the common and shared language between technical persons. “Radwaste” needs to consider the international literature before providing reports.

Geoscience is a multi-science discipline (thermal, geochemistry, geomechanic, geology, hydrogeology...) in relation with many other disciplines (safety assessors, engineering ...); the group recommends promoting inter-disciplinary communication within site characterisation teams.

Working Group C: Realities of Site Investigation

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Two examples of practical experience related to limits imposed by the practicalities of site characterisation were developed through the following presentations:

1. Spatial Extension and Parameter Integration into the Safety Case – Examples from the Hungarian LLW/ILW and HLW Disposal Projects by F. Fedor and I. Szűcs, (MECSEKERC Ltd., Hungary).
2. Complex Branching Structure in Crystalline Rock- Treatment of Uncertainty in Safety Assessment by J. Geier (Clearwater Hardrock Consulting, USA).

During the working session, Working Group C discussed the following questions proposed by the Scientific Programme Committee of AMIGO 2:

- *Provide a list of concrete examples of limitations and their reasons. In addressing these issues, consider the relation between what you can measure and what you would like to describe.*

  The working group members discussed the difficulties of obtaining distribution coefficient (K_d) values for radionuclides. From participants' experience, the determination of K_d values from *in situ* tests is generally more difficult than from lab tests due to the lack of precise knowledge of chemical conditions (e.g. Eh, pH) in the natural environment. Preference is generally given to lab tests because: (1) *in situ* determinations of sorbing processes require that the processes first be characterised/identified, (2) it is quite difficult to estimate the level of accuracy obtained from *in situ* tests, and (3) the results of *in situ* tests are generally not commensurate with the quality of the results of lab tests.

  The group also identified that *in situ* tests require much more time for their implementation than lab tests. In some cases, K_d values are needed before they can feasibly be obtained from *in situ* tests, leaving lab tests as the only viable option to collect the necessary data.

In some cases, the level of accuracy to be reached when determining the K_d value for a radionuclide is only that needed to demonstrate, with confidence, that the *in situ* or lab measurements are higher than a threshold value. This implies a strong link between the investigation programme and safety assessment (hypothesis and findings). For some working group members, maintaining consistency between the investigation programme and the safety assessment is a target in their programme. However, where a conservative approach is followed or required, which implies generally the use of simplified models coupled with deterministic conservative values, consistency is not necessarily a target. Best-estimate approaches, because they rely on more sophisticated models of chemical and/or physical phenomena, generally need more accurate input data.

Working group participants agreed that discussions and exchanges on the technical basis of limitations on obtaining data should be encouraged between implementers and regulators in order to develop an agreed upon line of approach.

- *Can these limitations be handled by defensible uncertainty descriptions?*

  Participants agreed that management of uncertainties is not an objective in and of itself. Management of uncertainties is a part of a global process that includes, at each step, a good understanding of the chemical and/or physical phenomena involved in the studied case. The amount of work involved in the management of uncertainties should also take into account how far away from the compliance limits a safety assessment is with the current level of uncertainty, and the stage the repository programme is at (greater uncertainty may be allowable during site characterisation than during licensing).

  How the management of uncertainties could be influenced by a conservative approach was also discussed. This way of working could be or is used in order to compensate for limitations resulting from a lack of data. However, the participants acknowledged that a conservative approach could introduce inconsistency between data or models (as, e.g. a parameter value that produces a conservative result when modelling one process may produce a non-conservative result when modelling a different process) and consequently could lead to a less comprehensive and understandable safety approach. In the case where a conservative approach is used, participants recommended assessing the level of conservatism introduced in the process because excessive conservatism could lead to unnecessary effort and expenditures.

  Participants pointed out that comparison between different models or methods can be a useful tool for identifying errors and for improving knowledge by understanding the possible differences in results. The use of global integrated modelling should be supported by a specific assessment of each separate field in order to increase the understanding of processes.

  Concerning site characterisation, participants recommended use of as realistic a model as possible. Simplifying or conservative assumptions can be made, as appropriate or necessary, during safety assessment, but should be avoided during site characterisation when a major goal is obtaining data and developing an understanding of mechanisms and processes.

- *What has been your experience in predicting properties/responses and then making comparisons with subsequent measurements? How much "after-fitting" was necessary? Did the exercise contribute to validation? What did it teach you about your abilities to characterise?*

  Positive and negative experiences about prediction capabilities were shared. A positive example could be found in the tracer tests that confirmed the prediction of the Boom clay sorption properties. Other examples come from mining experience, where high confidence in characterisation is obtained around a shaft, but the reliability of predictions diminishes with distance from the shaft. The presentation of R. Beauheim in plenary session 2 described probably the most common situation, where through an increasing number of boreholes (measurements), parts of the conceptual model were confirmed but, on the other hand, some fundamental hypotheses were not confirmed and had to be revised.

Participants recommended having as flexible a model as possible in order to be able to accommodate unexpected responses.

- *What are the realities of transferability of data between sites? What can actually be transferred (data, conceptual models, evaluation procedures) and what could not?*

  In addition to the presentation of M. Mazurek in plenary session 2, which constitutes an excellent framework of what could or could not be transferred and on what justification, participants agree that knowledge of process understanding and methods for site investigation and interpretation could be transferred. The transfer of geoscientific data, on the other hand, requires more of a case-by-case appraisal. Transferability applied to models should be strengthened by additional verification as, for example, the validity of assumptions. The concept of transferability could also be applied to experts. Exchange of experts could be envisaged in order to provide additional highly qualified and experienced human resources to a project.

  Extrapolation of information from a characterised area (URL) to the disposal area, which may be thought of as transferability inside the same site, should be done through a step-by-step approach. Measurements made during excavation of the disposal area should confirm predictions without unduly delaying the excavation process. Progressively, as these additional measurements confirm predictions, the number of measurements may diminish with time. Also, the stochastic nature of predicting geological properties or characteristics from remote or borehole-based investigations should be recognised in formulating the prediction exercise, so that deviations in details of measurements vs. predictions are not misconstrued as invalidating more general aspects of the models.

- *How have the experiences on possibilities and limitations influenced your investigation programme?*

  From feedback experiences, participants observed that cost-effective scheduling of many field activities (e.g. construction, drilling) is incompatible with the schedule for analysis and modelling activities, with the result being that modelling often lags behind characterisation activities. Moreover, modellers are often not confident enough in their results for modelling to be considered as an efficient tool to guide characterisation.

  Moreover, in some projects, the number of samples or amount of other data obtained is too small to support a full-scale model because for example, the confinement properties of the host rock should be preserved, or the property of interest could not be directly measured. In this case, surrogate or complementary understanding of geology could act as a substitute for data in developing models.

  Problems with long-term experiments have also been identified. Three mains factors that could jeopardise long-term experiment have been identified: the degradation of sensor reliability with time, the perturbations introduced by the monitoring system, and the costs associated with long-term experiments.

- *How are the limits in what can be achieved factored into safety assessment and engineering?*

  Participants acknowledged that the use of multiple lines of reasoning or a conservative approach in order to compensate for the inability to characterise a system fully should be a subject of discussion between the implementer and the regulator. During this discussion, the stage of the programme should be taken into account in such a way that the demands could be adapted to the limits of scientific capabilities or improvements. Sensitivity analyses could also be a useful tool to support multiple lines of reasoning.

Working Group D: Assembly and Integration of Geoscientific Knowledge and Arguments

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The purpose of this working group was to consider the assembly and integration of geoscientific knowledge and arguments.

In an introductory presentation, K. Skagius Elert presented “Assessment of Uncertainty and Confidence in Site Descriptive Models – Experience from the On-going Site Investigation Programme in Sweden”. The detailed description of concepts and procedures established at SKB for the development of a Site Descriptive Model (SDM) provided a starting point for the discussion of the working group. The SDM components and the procedures to achieve them were used as “references” for the discussion of comparable elements in other national programmes.

The observations have been placed into two broad themes:

1. How to manage the integration?
2. How to handle uncertainties?

No specific prescription was identified for either of these questions; rather a range of suggestions were noted based on experience. The appropriate solution will depend on the organisation, the site, the state of the programme, and other factors.

How to manage the integration?

Three general layers of geoscience information were identified, which can be loosely described as: site (point) data, discipline-specific models, and integrated description. For example, measurements of permeability in a borehole are point data. These are extended in space to form a permeability field in a hydrogeological model. Finally, this hydrogeological model is combined with information from geochemistry and other disciplines to form an integrated model.

The integrated model is often, e.g. in the Swedish programme, referred to as the Site Descriptive Model (SDM). Common attributes of this integrated model are that it is:

- controlled, e.g. version SDM 1.2;
- documented and traceable to the site data;

- a “best-estimate” description plus uncertainties – the use of conservatisms is left to safety assessors;
- a description of the site as it presently exists, e.g. without repository during the siting phase.

In parallel with the integrated description in the SDM, there may be a common controlled database. This ensures that all data used in the integrated description is consistent. For example, that the total porosity of the host rock matrix is the same in all disciplines (hydrogeology, geochemistry, rock mechanics). This requires that there be a central “clearance” or “acceptance” process for adding or changing information in the database. In the Nagra Opalinus Clay project, new data required that a document summarising the new value and its basis as well as its appropriate usage be prepared, and signed off by the data producer and the user (e.g. Geoscience and Safety Assessment representative) as a prerequisite for any usage of the data.

It should be noted that while there is conceptually a common database, in fact this may be structured as more than one physical database. In the SKB site characterisation programme, the SICADA database holds the site data (e.g. borehole logs), and the RVS and Simone databases hold the detailed model (SDM) information (e.g. reference discrete fracture network).

The process of managing the data and discipline-specific models, and integrating it into an SDM, involves communication and co-ordination. In principle, this can be viewed as human-oriented integration and code-oriented integration. Several formalised procedures (e.g. clearance protocols, workshop records) are implemented in national programmes in order to ensure this integration.

First, the development of an integrated site description requires that there be a process that involves input from technical experts representing the various technical geoscience disciplines. Given also the need for traceability of the model with data, this integration would typically be prepared through multidisciplinary reviews and workshops. For example, the formal process presently used by SKB as part of its site characterisation programme involves the following steps:

- assessment of the data – e.g. reliability, uncertainty, biases;
- quantify uncertainties;
- interaction matrix, to check process understanding, and in particular the interactions between processes;
- model consistency with past site evolution;
- changes from prior version of SDM are as expected.

Then, to the extent that there is an integrated code available with coupling of processes, this code can also be used to bring about integration of the site model. If different groups are using the same core model and database, then greater cross-discipline consistency of analyses and hypothesis (site model) testing is provided.

Ultimately, the involvement of numerous technical experts from different disciplines will require that there be a coordinating group. This would be a small group of people with both interdisciplinary skills as well as authority to make project descriptions relative to the development of the site model (both the modelling and the site characterisation activities).

Several other observations or suggestions were noted with respect to managing the integration:

- Iterate. Plan to conduct multiple iterations. Both within the geoscience group, as well as with safety assessment and engineering groups. Feedbacks from these groups are desirable already in the early stages – e.g. safety assessment needs might influence site investigation plans.

- Provide a common language. For example, it was observed that there are many different types of “porosity” used in models, and these should be clearly distinguished (e.g. transport porosity *versus* total porosity, or definitions of porosity by the method it was determined, e.g. water-loss porosity at 105°C). Another example was that geochemists had a different interpretation of “old” water than did hydrogeologists.
- Geology forms a common baseline to the site model. Hydrogeology and hydrogeochemistry form subsequent “layers”.
- Current “virtual reality” visualisation techniques can provide a useful tool to overlay datasets and explicitly compare datasets in the third dimension.

How to manage uncertainties?

Uncertainties in the integrated model must be formally evaluated and documented. This occurs at the various levels of integration noted earlier – the site data, the models, and the integrated site model.

For example, Box 1 below illustrates the questions asked at SKB as part of their formal process for assessing uncertainties in site data and related discipline-specific models.

Other processes to help identify or quantify uncertainties include:

- Evaluation by interdisciplinary workshop.
- Develop and evaluate alternative conceptual models (e.g. different fracture network, or Equivalent Porous Medium and Discrete Fracture Network models).
- Quantitative modelling (e.g. pdfs, ranges).
- Use of multiple lines of evidence and multidisciplinary discussion from other disciplines (e.g. “old” water signatures from geochemistry being used to constrain the rock permeability uncertainty).
- Consistency check with known features of the past evolution of a site,
- Feedback from the regulator and external reviewers (it is considered wise to plan to obtain such feedback early in the model integration process)

Processes that may be useful in helping to prioritise the uncertainties include:

- Feedback from safety assessment and engineering.
- Quantitative sensitivity analysis (e.g. may use Safety endpoints such as dose or risk as criterion of importance, and/or performance criterion such as the SKB Function Indicators). A more integrated and comprehensive model is better able to assess a wider variety of uncertainties, but simple models may be quite suitable in some cases.
- Use of 3-D visualisation techniques to better capture the dimensionality.
- Regulations, which may set context or provide guidelines for treatment of uncertainties (e.g. the use of 95th percentiles).

Handling of time evolution

A final observation from the working group was on the handling of evolution of the site with time. This topic incorporates aspects of both site integration and uncertainty management.

Specifically, the integrated site description model (SDM) noted above represents a description of the site as it presently exists. This description takes into account the site history, but does not describe its evolution. The latter involves a number of uncertainties.

This time evolution of the site can be described through Scenarios. The definition of scenarios, similar to the definition of the SDM, is an integrated and multidisciplinary process in order to ensure a self-consistent description. It will involve use of common assumptions. Since it involves the future and the associated uncertainties, it can be useful to draw on expert panels to help define the key assumptions and outlines for scenarios.

PART B

COMPILATION OF PAPERS

THE DEEP GEOLOGIC REPOSITORY TECHNOLOGY PROGRAMME: TOWARD A GEOSCIENCE BASIS FOR UNDERSTANDING REPOSITORY SAFETY

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1. Introduction

The Deep Geologic Repository Technology Programme (DGRTP) is advancing the geoscientific basis for understanding the safety of the Deep Geologic Repository (DGR) concept for long-term nuclear used fuel management (OPG, 2005). In this role, the DGRTP is fostering the development of geoscience methods and tools capable of generating an improved understanding of deep-seated Shield groundwater flow system evolution at time scales extending to 100 000 years and beyond. In part, this is being achieved through the development of illustrative case studies in which evidence is assembled to demonstrate concepts of flow system evolution and create a basis for a broader dialogue and consensus on geoscience and climate change issues that materially affect confidence in the predicted long-term performance of the DGR concept.

The Geoscience Work Programme is conducted through the coordinated efforts of 20 groups drawn from 10 Canadian universities, consultants, federal government organisations and international research institutions. Specific areas of investigation include Shield geology, structural geology, remote sensing, geostatistics, hydrogeochemistry, isotope hydrogeology, hydrogeology, paleohydrogeology, natural analogues, numerical methods, seismicity, long-term climate change (i.e. glaciation) and scientific visualisation. The work programme has been established to, among other issues, examine approaches for the integration and linkage of geoscientific reasoning that attempt to constrain inherent non-uniqueness and uncertainty associated with the interpretation and prediction of Shield flow system dynamics and evolution at time scales relevant to DGR implementation. Through this approach, an improved fundamental understanding of Shield flow system evolution and applicability of techniques to communicate this understanding are being developed.

Determining the suitability of a specific site will require an assessment of geosphere stability. Stability has broad meaning that includes both repository engineering considerations, and the geosphere processes and mechanisms that govern subsurface groundwater flow and mass transport. One aspect of stability relates to the resilience or constancy of the groundwater flow system to foreseeable change in flow system property distributions, transient boundary conditions or both. An example would be that of glaciation, which during the latter half of the Pleistocene epoch markedly altered the landscape of the Shield through cyclic periods of temperate, boreal, peri-glacial, then ice-sheet cover and retreat on an approximate 100 000 year timeframe.

The response or behaviour of the geosphere with respect to long-term change is determined by factors such as site-specific fracture or discontinuity frequency, orientation, geometry and inter-connectivity, variable groundwater salinity, watershed topography and permeability distributions within rock mass volumes that exceed several km^3. Unique transient boundary conditions and site characteristics will govern to a certain extent the migration of environmental isotopes, hydrogeochemical flow system signatures, fracture infill mineral assemblages, as well as groundwater flow pathways and the depth of penetration by oxygenated glacial recharge – all related points that either through consistency in interpretation or occurrence contribute to knowledge regarding geosphere barrier integrity and long-term stability. A key goal in the DGRTP is the development of tools with improved utility to explore and communicate how such foreseeable long-term events and site-specific geologic features affect confidence in the prediction of long-term geosphere barrier performance.

This extended abstract provides an overview of the factors or motivation for development of the DGRTP Geoscience Work Programme and specific selected activities that illustrate projects and new methodologies fostered within the work programme to advance the geoscientific basis for understanding Shield groundwater evolution as relevant to the safe implementation of the DGR concept.

2. DGRTP geoscience work programme: approach in design

The development and coordination of individual DGRTP Geoscience work programmes is guided by several key factors. These are:

i) *Descriptive Conceptual Geosphere Model:*

   An emphasis is placed on co-ordination of work programmes to improve clarity and transparency of the geoscientific evidence and logic that supports the development of an integrated, site-specific, multi-disciplinary, descriptive, conceptual geosphere model (Jensen and Goodwin, 1999). This process serves several roles within the DGRTP including: a) a systematic framework to assemble and test flow system hypotheses; b) a forum in which multi-disciplinary groups are engaged to understand how their data influence confidence in the descriptive and predictive model outcomes; c) a basis to constructively convey a sense of data worth to investigators who might not otherwise appreciate the utility of their information; and d) a method to demonstrate to site characterisation groups improvements in methods of data collection, and/or interpretation that best serve to instil confidence in predictive estimates of DGR performance.

ii) *Deep Seated Flow Domain:*

   The Geoscience programme aims at developing tools and multiple lines-of-reasoning for advancing the understanding of physical and chemical stability of deep flow systems (500-1 000 m) in fractured-porous media at time scales of 100 000 years. This includes the development of tools and methods applicable in either crystalline or sedimentary rock settings.

iii) *Non-Uniqueness:*

   In geoscience, non-uniqueness is problematic. Current work programme activities and new initiatives are directed toward addressing issues of spatial and temporal uncertainty such that the robustness in predictions can be best demonstrated. Further, this approach is developed recognising practical limitations during DGR investigations on the ability of site characterisation techniques and methods to allow complete or unique characterisation of required rock mass volumes.

iv) *Multiple Lines of Reasoning:*

   Based on non-uniqueness, a process is required to ensure that multi-disciplinary evidence is used to constrain both the conceptual descriptive geosphere model(s) and predictive numerical realisations for flow or mass transport. In this regard, it is important to demonstrate how reasoning independent of modelling (i.e. paleohydrogeology; isotopic flow domain systematics, hydrogeochemistry; natural analogue investigations) can enhance confidence in predictive outcomes.

v) *Peer Review:*

Independent technical peer review is an important aspect of the Geoscience Work Programme. Peer review serves two primary roles: a) it provides for open communication with the geoscientific community to solicit candid feedback; and b) it maintains and fosters technical credibility in the DGRPT Geoscience programme.

3. Shield groundwater flow system evolution: case study

As previously discussed, one specific goal of the geoscience work programme is associated with assembling geoscientific evidence to advance the understanding of groundwater flow system evolution and dynamics during the Quaternary period within deep-seated regional (≈5 000 km^2) and local scale (≈100 km^2) Shield settings. This involves a multi-disciplinary approach that is intent on providing a structured and systematic framework to reveal: i) the relative importance of site-specific flow domain property attributes and geometry, and boundary conditions on flow domain stability; ii) the impact of site characterisation uncertainty with respect to realisation of property distributions and boundary conditions; and iii) geoscientific indicators of stability that foster reasons for confidence or otherwise in the repository Safety Case.

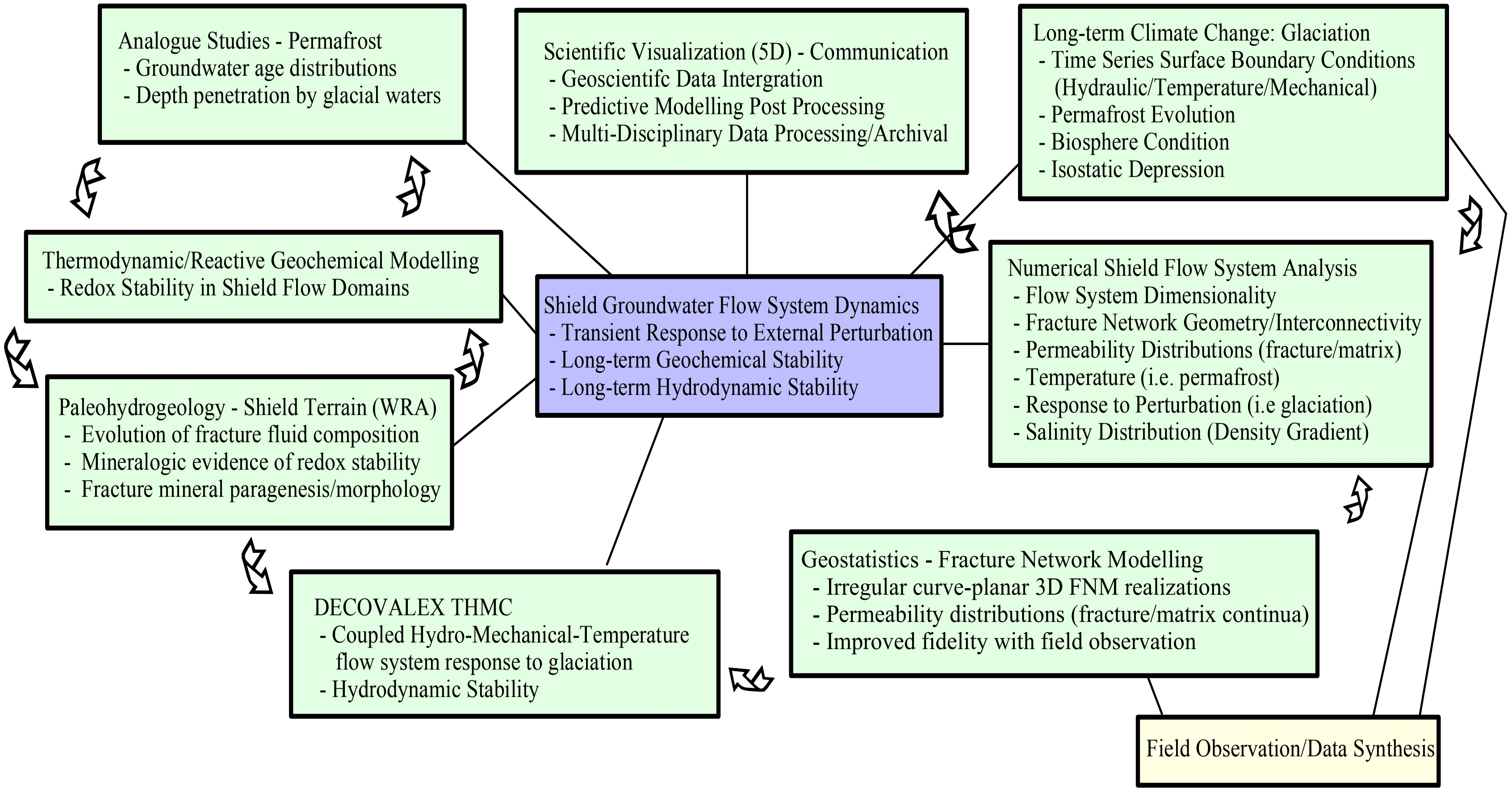
In order to constrain the understanding of flow system evolution, the approach adopted involves developing multiple-lines-of-reasoning with respect to processes and mechanisms contributing to an understanding of long-term flow system stability (Jensen and Goodwin, 2003). In so doing, work programme activities have been purposely linked or aligned such that collectively they create a means to communicate aspects of Shield flow system evolution (Figure 1). Within the following 3 sub-sections, work programme examples have been drawn from Figure 1 to illustrate activities within the DGRTP that are contributing to a means to constrain uncertainty and non-uniqueness in geoscientific understanding, as well as a systematic and structured framework within which to explain the derivation and assembly of a site-specific descriptive conceptual geosphere model.

3.1 Regional and sub-regional shield flow system simulations

The programme activities during 2004 focused on numerical simulations at the local or sub-regional flow system scale (Sykes *et al.* 2004). The model applied was a hybrid, discrete-fracture, dual continuum realisation of the finite element model FRAC3DVS. The modelling approach included use of a realistic Digital Elevation Model (Fracture Network Model (FNM) that honoured many site-specific geological, statistical, and geomechanical constraints DEM) of the flow domain's topography, the explicit discretisation of a 3-dimensional, curve-planar, (Srivastava, 2002ab, 2003, 2004), and the use of fine discretisation grids that improved upon the previous studies of a similar nature.

As part of the analysis, a single realisation of the complex sub-regional FNM was superimposed onto a 600 000 element FRAC3DVS flow domain mesh. Orthogonal fracture faces (between adjacent finite element blocks) were used to approximate the irregular FNM comprised of more than 540 individual discontinuities. The crystalline rock mass between these structural discontinuities was assigned a range of properties considered characteristic of Shield terrain. Simulation results that reveal and capture the complex distribution of Darcy fluxes within one realisation of the flow domain are shown in Figure 2. In all of the simulations performed, predicted Darcy fluxes at depths below approximately 600 m are indicative of mass transport regimes in which diffusion would be the dominant transport mechanism. Future work programme activities will be devoted to coupling

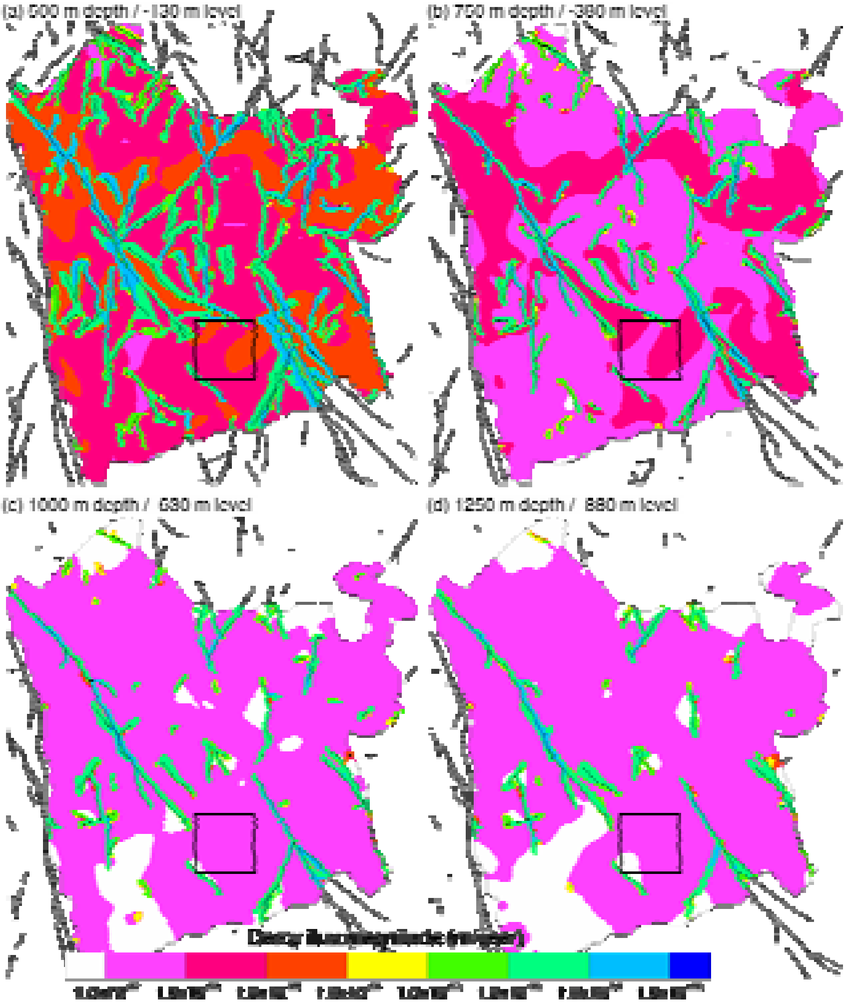
Figure 1. **Multiple-lines of Reasoning and Linkage of DGRTP Geoscience Programmes to Develop a Geoscientific Basis for Repository Safety.**



sub-regional flow system simulations with transient long-term climate change surface boundary conditions, uncertainty analysis to incorporate multiple and equally probable FNM realisations, groundwater salinity and spatially-correlated permeability fields in both fracture and matrix continua. The intent is to advance the utility of FRAC3DVS to enable a more rigorous and complete assessment of flow domain uncertainty as it affects the potential siting and development of a Safety Case for a DGR within a crystalline or sedimentary rock environ.

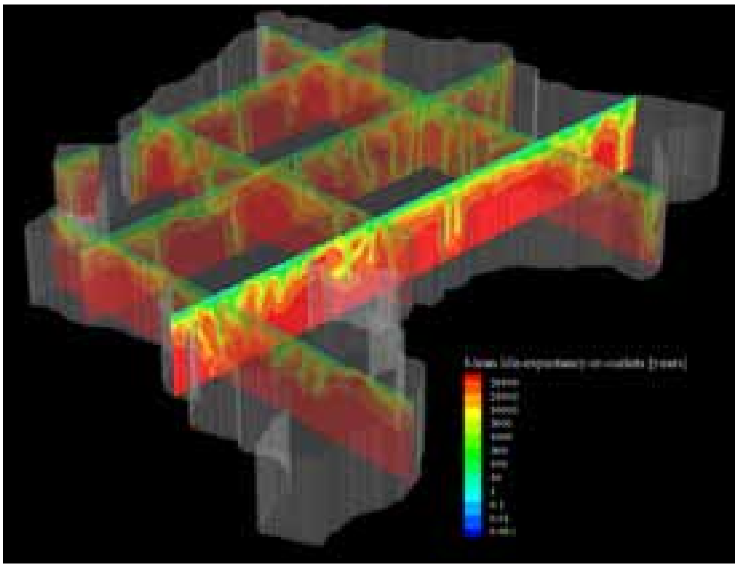
Further activities related to improving the utility of predictive tools have involved the implementation of a Time Travel Probability technique within FRAC3DVS. This technique involves the solution of the advection-dispersion equation to derive Probability Density Functions (PDFs) that represent the statistical occurrence of water particles with respect to time as a consequence of mixing processes. Such PDF's can be representative of groundwater age (time since recharge) or life expectancy (time to discharge). This technique can preserve site-specific flow system dimensionality, fracture network geometry, permeability distributions and contrasts, salinity distributions and time varying boundary conditions. An example that illustrates predicted mean life-expectancy for a single realisation within the aforementioned sub-regional

Figure 2. **Predicted distribution of groundwater Darcy fluxes at selected depths within a representative sub-regional Canadian Shield flow domain, based on 3-dimensional, steady-state, freshwater, numerical simulations FRAC3DVS (Sykes *et al*. 2004).**



flow domain is shown in Figure 3. This innovative technique is beginning to provide a further basis to understand and provide reasoned visualisation of the magnitude of uncertainty in computed age determinations as affected by flow system properties and boundary condition uncertainty. In so doing, it is yielding a constructive means to explore and illustrate coincidence with other site characterisation field data sets, for example hydrogeochemical or environmental isotope distributions, with the intent of fostering confidence in knowledge of bounds on flow system behaviour.

Figure 3. **Mean Life Expectancy (time to discharge) for the sub-regional flow domain based on implementation of the Travel Time Probability technique within FRAC3DVS. Results are based on a single, steady-state, fresh-water realisation of the sub-regional flow domain as described in Sykes *et al.* (2004).**



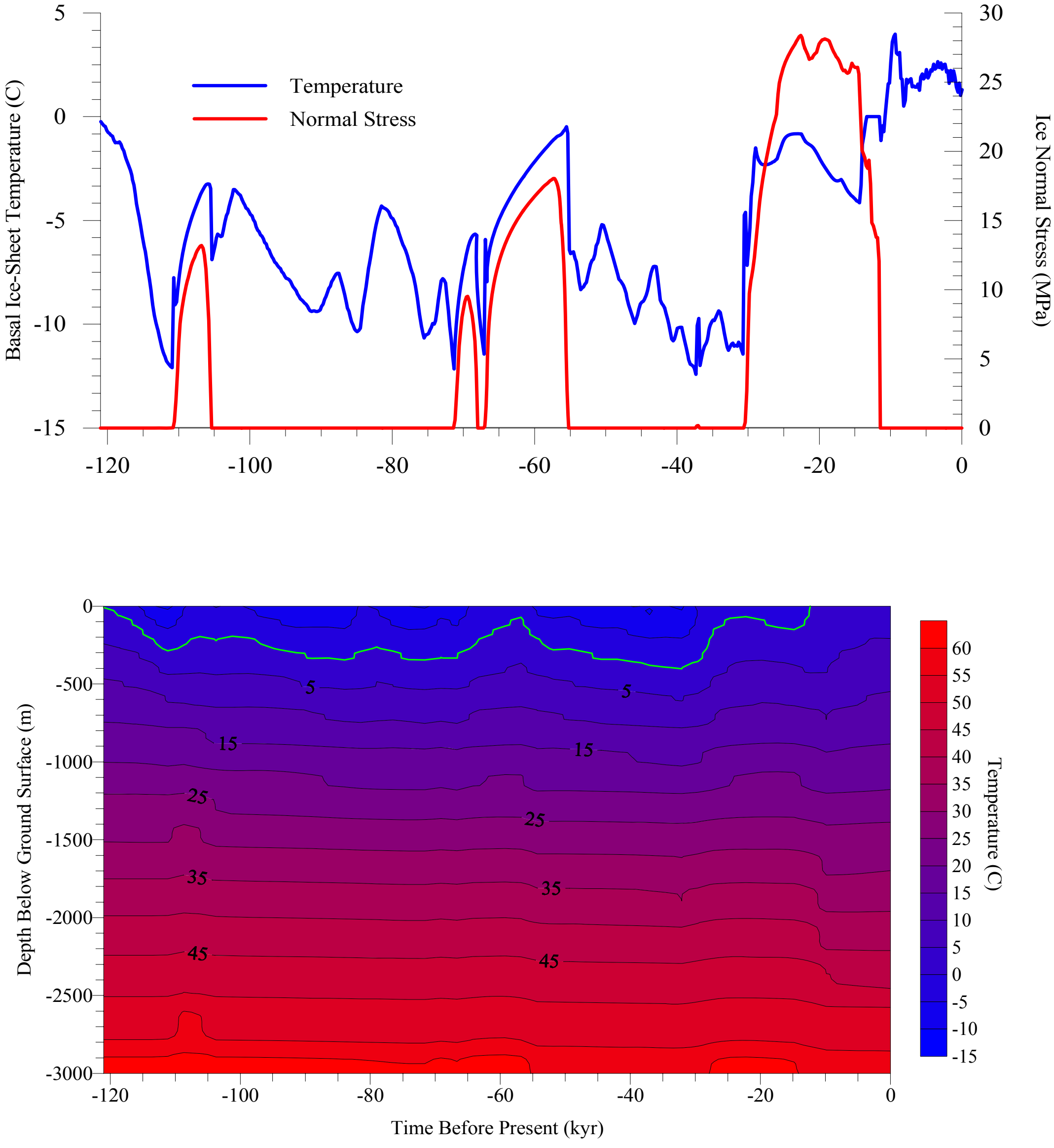
3.2 *Long-term climate change – glaciation and permafrost*

Within the northern latitudes of Canada, the performance of a DGR for used nuclear fuel at depths of 500 to 1 000 m within the crystalline rock of the Canadian Shield will be affected by long-term climate change. As surface conditions are predicted to change from present day boreal to peri-glacial, variable ice-sheet thickness cover and then rapid glacial retreat (8-10 kyr), coincident transient geochemical, hydraulic, mechanical and temperature conditions will be imposed on the Shield flow system.

With respect to understanding Shield groundwater flow system dynamics and stability, an important consideration is the influence of the gradual or episodic nature of such transient boundary conditions on, for example, the magnitude and rate of change in groundwater flow rates/directions, the depth of penetration and mixing of surface-fracture-matrix end member waters, depth of redox front migration and changes in rock stress magnitude and orientation.

Work programme efforts related to furthering the understanding of long-term climate change and glaciation have focused on advancing climate-driven, predictive estimates of the last continental glaciation with the University of Toronto Glacial Systems Model (GSM). These simulations yield geophysically constrained estimates of Laurentide ice-sheet geometry, advance and retreat, ground surface temperatures, basal ice-sheet meltwater fluxes, glacial isostatic depression and, more recently, permafrost evolution. An example of the complex and dynamic nature of surface and permafrost conditions reasonably expected to influence a hypothetical Shield site is shown in Figure 4. This figure depicts one realisation of the GSM that predicts ground surface temperatures, ice-sheet normal stress (equating to ice-sheet thickness) and coincident ground temperature changes to depths of 3 km. Although preliminary in nature, these latter estimates yield plausible approximations of freezing depths as constrained by an understanding of the current occurrence of permafrost and coincidence with time-series ground surface temperature data derived through inversion of deep borehole temperature logs from 4 Shield locations. A more detailed description of the GSM model and the methodology applied to predict ground temperatures and permafrost evolution are provided by Peltier (2003) and Peltier (2004), respectively.

Figure 4. **University of Toronto Glacial Systems Model – prediction of Laurentide ice-sheet and permafrost evolution at a representative Canadian Shield site: a) time-series estimates of ground-surface temperatures and normal stress (ice-sheet thickness); and b) time-series estimates of ground temperatures depicting depth of freezing point (permafrost) during glacial cycle.**



3.3 Scientific visualisation

A DGRTP work programme was initiated at MIRARCO, based at Laurentian University, to explore the utility and application of Scientific Visualisation supporting the integration, validation, visualisation and communication of complex numerical modelling results associated with the development of the conceptual geosphere model for the next generation sub-regional (100 km^2) Shield flow system and the evolution of this flow system as affected by long-term climate change. New advanced visualisation techniques are being developed to facilitate the querying, interpretation and integration of: i) multiple, geostatistically-simulated, fracture network model (FNM) realisations that form the basis for the geosphere model used as input to FRAC3DVS; ii) geostatistically-generated permeability fields associated with the fracture networks and the rock domains between the fractures to depths of 1 000 m; iii) the FRAC3DVS model grids, as well as the results of transient simulations of groundwater flow evolution (Darcy fluxes, pressure head changes, groundwater residence times, salinity changes etc.) as a function of alternative FNMs and spatially variable permeability fields; iv) the influence of coupled climate/surface boundary conditions associated with a Laurentide glaciation scenario on the abovementioned simulations; and v) the linkages to multi-disciplinary data sets (e.g. hydrogeochemical and isotopic data) that help to constraint/support the above modelling results.

Ultimately, the main goal of this work programme is to develop an approach to data integration and communication that facilitates the understanding of the role and importance of flow system characteristics and evolution pathways that control mass transport in sub-regional scale Shield environments. This goal will be facilitated within a collaborative, immersive, virtual reality environment, where ideally “the data should speak for themselves”.

4. Summary

Within the Deep Geologic Repository Technology Programme (DGRTP) several Geoscience activities are focused on advancing the understanding of groundwater flow system evolution and geochemical stability in a Canadian Shield setting as affected by long-term climate change. A key aspect is developing confidence in predictions of groundwater flow patterns and residence times as they relate to the safety of a deep geologic repository for used nuclear fuel waste. This is being achieved through a coordinated multi-disciplinary approach intent on: i) demonstrating coincidence between independent geoscientific data; ii) improving the traceability of geoscientific data and its interpretation within a conceptual descriptive model(s); iii) improving upon methods to assess and demonstrate robustness in flow domain prediction(s) given inherent flow domain uncertainties (i.e. spatial chemical/physical property distributions, boundary conditions) in time and space; and iv) improving awareness amongst geoscientists as to the utility of various geoscientific data in supporting a safety case for a deep geologic repository.

This multi-disciplinary DGRTP approach is yielding an improved understanding of groundwater flow system evolution and stability in Canadian Shield settings that is further contributing to the geoscientific basis for understanding and communicating aspects of DGR safety.

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LONG-TERM CLIMATE CHANGE: THE EVOLUTION OF SHIELD SURFACE BOUNDARY CONDITIONS

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1. Introduction

The Earths surface during the Pleistocene epoch has been repeatedly subjected to glacial cycles that have markedly influenced both the landscape and surface boundary conditions that, in part, governed past evolution of deep-seated Shield groundwater flow domains. As part of the Deep Geologic Repository Technology Programme simulations of the last Laurentide glacial episode have been undertaken with the University of Toronto Glacial System Model (GSM). The purpose of these simulations is to yield constrained predictions of the magnitude and time rate of change of peri-glacial, glacial and boreal regimes that have perturbed Shield flow domains in the geologic past. On the basis of the fact that the North American continent has been re-glaciated approximately every 100 000 years over the past million years of Earth history it is strongly expected such glacial events would and could potentially influence the performance of a used nuclear fuel repository. Recent significant advances in the ability to quantitatively assess the transient variations in surface boundary conditions that such an event would involve, and to assess the degree of non-uniqueness that is inevitably involved in such an assessment, are now being applied to allow a more complete assessment of the influence that long-term climate change may impose on a future hypothetical Shield repository site. This paper describes these advances and provides an illustrative example of how this is contributing to an improved basis for understanding the role of long-term climate change in affecting Shield flow system evolution and impacts on repository performance.

2. Background: glacial systems model – approach

A series of analyses has been performed in order to provide a detailed understanding of the expected magnitude and time rate of change of surface boundary conditions occurring during a Laurentide (North American) glacial cycle. These analyses were performed with the University of Toronto Glacial Systems Model that has been developed over the course of the past decade (Deblonde and Peltier 1991, 1993; Tarasov and Peltier 1997, 1999, 2002, 2004). The current version of the model includes a 3-D thermo-mechanically coupled ice sheet model, a bed thermal model that extends to a depth of several kilometers and which may be employed to predict the occurrence and evolution of permafrost depth, a sub-glacial till deformation model, a temperature dependent positive degree day mass-balance model with a physical refreezing parameterisation, a spherically symmetric visco-elastic isostatic response model (e.g. Peltier, 2005) and a fast drainage routing solver that may be employed to accurately determine the routing of meltwater to the sea produced during episodes of deglaciation (Tarasov and Peltier, 2005).

A key input to the GSM concerns the climate forcing that is assumed to operate during the process of ice sheet advance and retreat. In accord with the current state-of-the-art in this area, the

GRIP ice core derived DEL18O record is used to define the time variation of surface climate (temperature and precipitation) as a means to interpolate between a glacial maximum climate determined by an average of an ensemble of the highest resolution subset of the models developed in the context of the international PMIP collaboration, and a modern climate determined on the basis of the NCAR/NCEP reanalysis project. Because the millennial scale variations of the extent of glacial cooling revealed in the GRIP core are expected to be of at least hemispheric scale, it is expected that this methodology should deliver a reasonable approximation to the climate variability that actually forces the advances and retreats of glacial ice.

A crucial aspect of the analyses that have been performed has involved the computational apparatus designed to aid in the assessment of the uniqueness of the time dependent boundary conditions that are inferred on the basis of the GSM. This aspect of the analysis involves an extensive Bayesian calibration of the model against a wide range of geophysical constraints to ensure that the model accurately reproduces, within observational error, the variations in observables that characterise the aftermath of the most recent Laurentide glacial cycle. Because the model is expensive to run, a neural network which may be employed to emulate the statistics that it generates has also been developed with which it has been possible to extensively probe the phase space of solutions to the nonlinear problem of ice sheet advance and retreat so as to ensure that predictions are not trapped in a local and non-physical equilibrium. Using this apparatus it is possible to provide a rigorous assessment of the issue of non-uniqueness which is critical in bounding a possible range of event outcomes.

3. Predictions of long-term climate change

An illustrative example of the evolving thickness of the Laurentide Ice Sheet (LIS) during a typical 100 000 year glaciation and deglaciation cycle, as predicted with the GSM is depicted in Figure 1. The results illustrated in Figure 1 are drawn from a simulation that was strongly constrained so as to enable the model to reconcile independent time-series of geophysical, geological and geodetic data that may be brought to bear on the problem. The individual time slices shown are those for a sequence of times in the deglaciation phase of the cycle that began approximately 20 000 years ago. The data employed to constrain the calculation include ^{14}C dated relative sea level histories, ice margin positions as a function of time through the deglaciation phase of the ice-age cycle, and geodetic observations of the present day rates of vertical motion of the land based upon absolute gravity measurements or measurements based upon the application of Very Long Baseline Radio-Interferometry (VLBI). Also shown on this Figure are the predicted locations of the pro-glacial lakes that are known to have formed during the retreat phase of the ice-age cycle. It is a characteristic of all such models of the process that fit the totality of the available data (e.g. Peltier, 2004) that the present Hudson Bay is a local minimum of ice thickness at the Last Glacial Maximum (LGM) 21 000 years before present. This is a consequence of the continuous action of the Hudson Strait Ice Stream during the glacial period, a feature of the LIS that acted so as to “draw down” the maximum in thickness over this region that would otherwise form.

Of particular interest from the perspective of repository safety is the evolution with time of the depth extent of permafrost that would have existed during the cycle of glaciation and deglaciation. The GSM is designed to make rather accurate predictions of this sub-surface manifestation of glacial advance and retreat when sufficiently high vertical spatial resolution is employed to describe the subsurface thermal regime. Figure 2 shows a sequence of maps of the predicted thickness of permafrost on the North American continent as a function of time through the glacial cycle. The times selected for presentation in this case are for a sequence of widely spread times that lead up to the time of the maximum of glaciation. Notable is the fact that during the inception phase of the cycle during which the LIS is expanding there is predicted to exist an extensive “halo” of permafrost surrounding the advancing ice sheet. Under the ice sheet itself, however, the surface of the Earth is predicted to be at or very close to the pressure melting point of the overlying ice, a consequence of the insolating effect of the ice sheet which acts so as to trap the heat flowing into the base of the ice sheet from the solid Earth. The quality of these predictions of the model may be assessed by comparing the present day permafrost depth predictions to field observations over the continent, a test that the model passes with reasonable accuracy, especially considering that permafrost depth has been approximated simply as the depth to the 0°C isotherm, thereby neglecting the impact that might be expected due to the finite salinity of pore waters. It has also proven possible to test the quality of this prediction of the model for times other than the present by making use of ground surface temperature inferences for earlier times derived from the formal inversion of borehole temperature records (e.g. Rolandone *et al.* 2003). Their inferences of surface temperature for LGM at several sites in Manitoba and Quebec are also in close accord with the predictions of the UofT GSM.

Figure 1. **Deglaciation chronology and meltback sequence for the high velocity model from the ensemble that best fits the totality of the observational data over the time interval from 20,000 calendar years before present and 8 000 calendar years before present. The Figure also shows the time dependent ice-thickness as well as theproglacial region that is expected to be water covered during the retreat phase.**

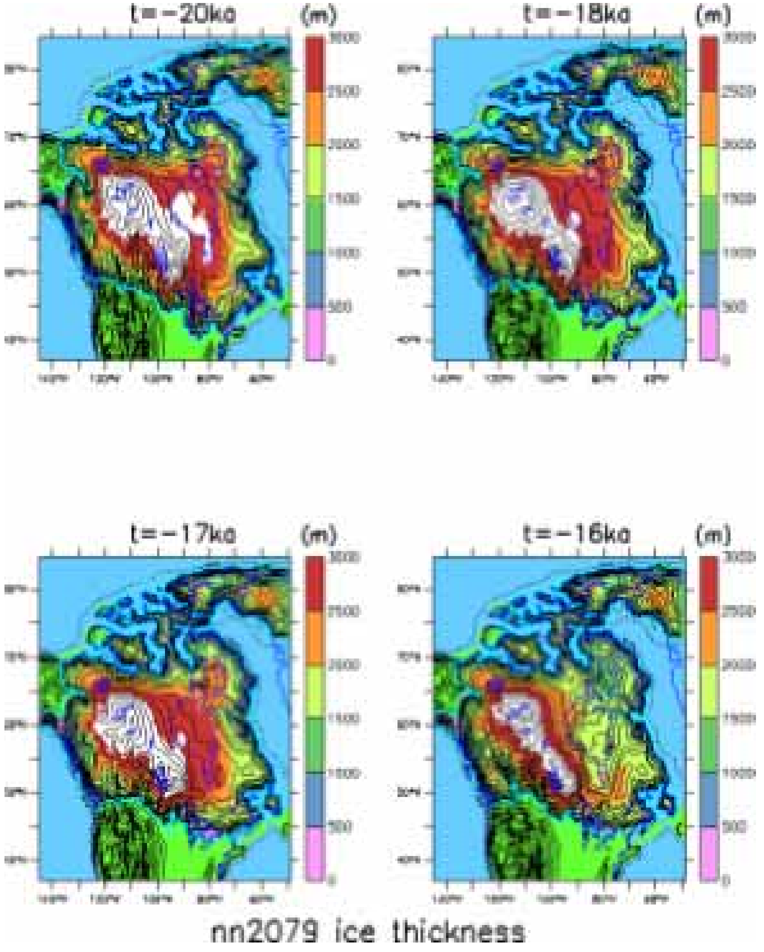
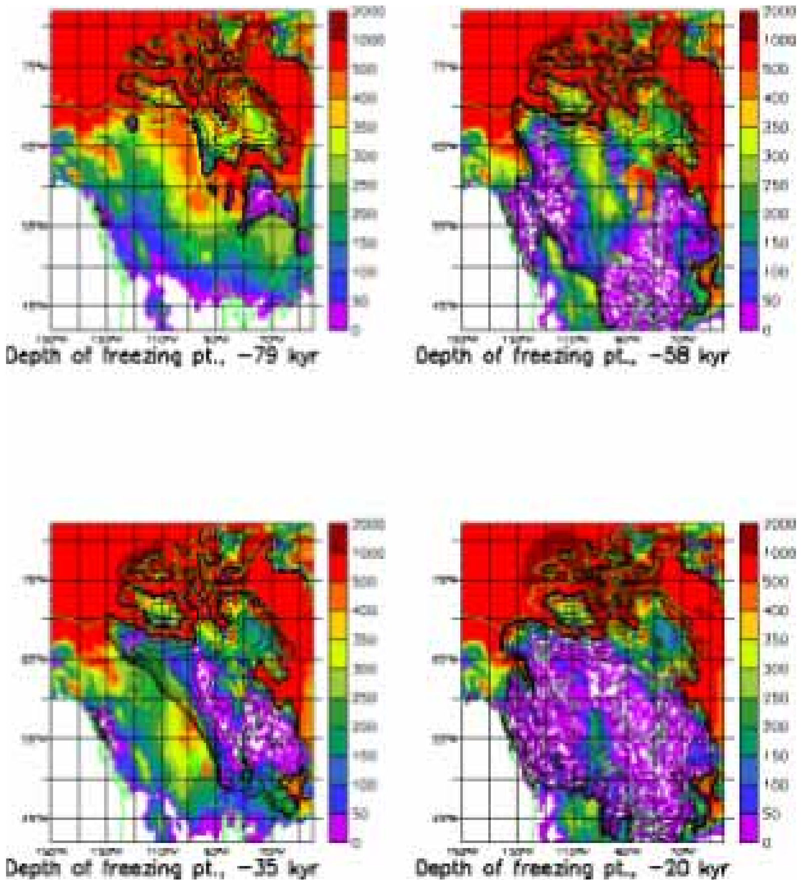


Figure 2. **Permafrost depth as a function of time over the entire North American continent from a typical version of the 100 kyr ice-age cycle as represented by the University of Toronto Glacial Systems Model. The colour bars represent depth of penetration of permafrost in metres.**



4. Summary and Conclusions

A detailed model of long timescale climate change has been developed, the University of Toronto Glacial Systems Model, which is able to make useful predictions of the process of continental glaciation and deglaciation that has occurred in the past due to the small changes in the effective intensity of the Sun at the location of the Earth caused by gravitational many body effects in Solar System evolution. Based upon the success of this model we are able to assert that we have demonstrated a basic understanding of why this process has continually recurred in the past on a timescale of approximately 100 000 years. Continuing work with the Glacial Systems Model and efforts to provide explicit linkage to numerical analyses of sub-surface hydrology are beginning to yield a new understanding of groundwater flow system evolution and response to glacial perturbations. In so doing this understanding is not only providing a reasoned basis on which to examine issues of geosphere stability as relevant to the safety of a hypothetical repository for used nuclear fuel in Shield terrain, but is also offering an improved basis for the integrated interpretation of multi-disciplinary geoscientific data necessary for development of a descriptive geosphere model that is seen as fundamental to the repository Safety Case.

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FRACTURE NETWORK MODELLING: AN INTEGRATED APPROACH FOR REALISATION OF COMPLEX FRACTURE NETWORK GEOMETRIES

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1. Introduction

In its efforts to improve geological support of the safety case, Ontario Power Generation's Deep Geologic Repository Technology Programme (DGRTP) has developed a procedure (Srivastava, 2002) for creating realistic 3-D fracture network models (FNMs) that honour information typically available at the time of preliminary site characterisation:

- Detailed information on the locations of surface lineaments, which is typically available from aerial photography, remote sensing or ground reconnaissance.
- Regional tectonic information on stress, which can often help to constrain the style of fracturing: dominantly low-angle features in compressional regimes, dominantly sub-vertical in tensional regimes.
- Geomechanical and structural geology principles, which may assist with predicting down-dip behaviour of fractures.
- Field data gathered from geologically analogous sites, which may provide supporting information on fracture density, orientation and truncations.

2. Methodology

Sequential gaussian simulation (SGS) is a geostatistical procedure widely used for creating data-conditioned stochastic models of spatial phenomena. In a typical SGS study, the procedure is applied on a regular grid to volume-averaged rock properties. In the procedure discussed here, SGS is applied to geometric attributes – strike and dip of fracture surfaces – on an irregular grid whose nodes are determined iteratively as the procedure progresses.

The original motivation for using an iterative procedure like SGS was to mimic the procedure proposed by Renshaw and Pollard (1994). Their approach to 2-D fracture simulation was based on geomechanical principles, propagating fracture tips when stress exceeds a critical threshold. Their approach gives realistic synthetic images of fractures in a variety of stress environments, displaying many subtle features commonly observed in the field, such as zones of small *en échelon* cracks that bridge gaps between larger sub-parallel fractures.

Though undeniably successful, fracture simulation based on geomechanical principles proved to be computationally prohibitive and has not yet been extended satisfactorily to 3-D. By using the same broad approach – an iterative procedure for propagating fracture tips – but replacing geomechanical principles for fracture propagation with geostatistical rules, one is able to mimic much of the realism with considerably less computational effort.

The simulation of the fracture networks is handled in two steps. First, the surface traces of the fractures are propagated in 2-D to create a complete rendition of the fracture network at surface. Second, the surface traces are propagated to depth.

For the surface propagation of the fracture traces, SGS is used to simulate the azimuth or strike direction of the traces. Each fracture trace begins as a seed point that belongs to a certain direction class and is assigned a target length. From this initial seed point, the fracture is propagated in either direction following the usual SGS approach: i) nearby data (which include actual observed fractures as well as stochastically simulated ones) are used to estimate a local distribution of possible azimuths for the next segment; ii) this distribution is sampled to produce a specific azimuth and the fracture trace is then extended in that chosen direction.

One of the input parameters is a table of truncation probabilities that is used to decide what happens when two fractures meet. This table provides the probability that a fracture from group i will truncate against a fracture from group j. If the i, j truncation probability is set to 1, then a fracture from group i will terminate against a fracture from group j whenever they meet; this type of behaviour is appropriate for faults, with older faults truncating against younger ones. If the truncation probability is set to 0, then the fractures can cross each other; this type of behaviour is appropriate for joints. Intermediate values between 0 and 1 allow the user to control the style of truncations from more joint-like to more fault-like.

Once the surface traces have been simulated, the propagation to depth is performed, again using SGS. Each line segment in 2-D is propagated down-dip by simulating a dip angle (constrained by surrounding data) and adding a triangular facet that follows this simulated dip. Down-dip propagation is terminated either when fractures truncate against other fractures, or when they reach a target width calculated from a length-to-width assumption.

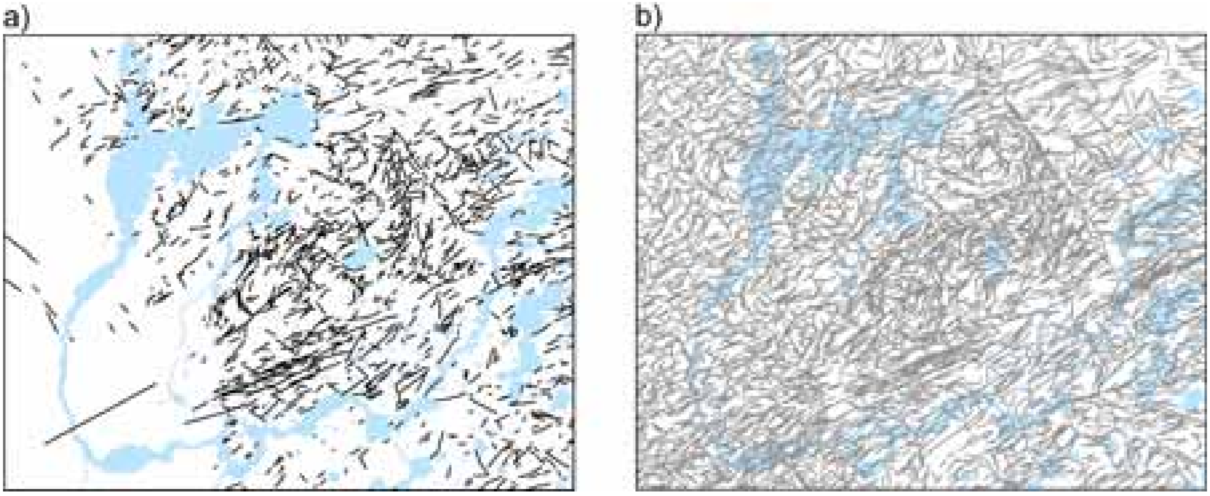
3. Case study applications

3.1 Whiteshell research area

The surface lineament database for AECL's Whiteshell Research Area (WRA) served as the basis for the first DGRTP application of this approach to fracture network modelling.

In regions where ground cover and lakes limit the exposure of visible lineaments, the fracture density is under-represented in the lineament data base. In these areas, the fracture network models extend the mapped lineaments and add additional stochastic lineaments to bring the fracture density to the level seen in areas of good bedrock exposure. Figure 1a shows an example of the identified fracture traces for the WRA; fractures are less numerous in the west, where the floodplain of the Winnipeg River makes it difficult to detect lineaments. Figure 1b shows an example of the simulated fracture network at surface, with stochastic lineaments having been added in regions with poor bedrock exposure and the features from Figure 1a being retained in regions with good bedrock exposure.

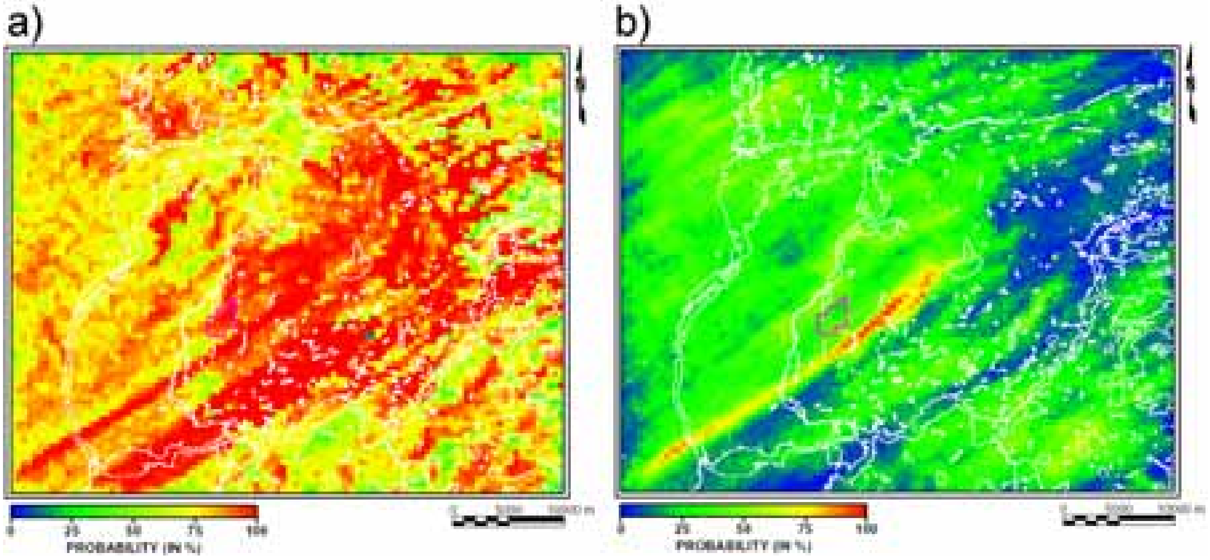
Figure 1 a b. **Examples from Whiteshell Research Area case study. The fracture traces identified from various sources of remote sensing data in 1a) under-represent the true fracture density in the west. The simulated fractures in 1b) honour the data in 1a) and in-fill stochastic features in areas where lakes and fluvial sediment cover obscures the underlying fractures.**



Knowledge of the tectonic history of the study area was used to make reasoned judgements about the down-dip nature of the fractures, with the Lac du Bonnet batholith being dominated by low-angle fractures typical of a compressive environment.

Using only the available surface data, a set of 100 FNMs was created and used to calculate the probability of intersecting a fracture at depth. The results (Figure 2) show a clear decrease in the chance of hitting a fracture as depth increases, a feature of the geosphere that has been confirmed by sub-surface investigations at the WRA and other Canadian Shield sites.

Figure 2 a b. **Probability of intersecting a fracture at depths of 300-350m (2a) and 800-850m (2b).**



3.2 Sub-regional flow model

A region of typical Canadian Shield has been selected as a test case for the DGRTP's ability to model the geosphere. A fracture network model of this region has been built, using prominent lineaments from aerial photography as the deterministic fractures at surface, and adopting fracture length and density statistics from the Whiteshell Research Area.

100 realisations of the 3D fracture geometry were created to explore the use of the probabilistic information provided by the geostatistical simulations in flow and transport modelling.

The results of this exercise confirm that the detail and geometric complexity of the simulated fractures can be successfully imported into FRAC3DVS, a finite difference flow and transport simulator. Automated procedures for incorporating the fracture surfaces allow the rapid importation of the entire suite of alternate FNMs, which enables risk analysis to include effects due to the uncertainty on fracture network geometry.

3.3 Lägerdorf case study

The Lägerdorf data set consists of highly detailed maps of fracture traces for twelve parallel faces of one wall of the quarry as it was advanced in small increments (roughly 1 to 1.5 metres). Each face map spans a region approximately 230 metres long by 40 metres high. All sections are inclined at approximately 50º. The faces were available for mapping during production, where the excavation process continuously scrapes a layer of 1.5 m thickness off the wall of the quarry by an abrading conveyor belt. During the period of the mapping programme, the quarry wall was advanced 25 metres. The set of twelve face maps therefore represents a high resolution 2½-D fracture data set of a 230x40x25 m volume.

To test the SGS-based geostatistical procedure for fracture network simulation, the stack of parallel face maps was rotated so that the walls are essentially horizontal, with Wall 1 being at the top and Wall 12 being at the bottom. By doing this rotation, we are able to treat data from Wall 1 as a set of deterministic "surface" fractures that will be used as conditioning data for a simulation of 3-D fracture geometry. In order to make the test as illuminating as possible, all data from Walls 2 through 12 were ignored. Once a set of simulations of 3-D fracture geometry was developed, each realisation was sliced along the planes corresponding to the walls not used as conditioning data and the resulting simulated face map can be compared to the actual face map for each wall.

This verification exercise confirms that the geostatistical procedure for fracture simulation not only honours primary fracture statistics, such as fracture length and orientation distributions, but also successfully reproduces many more subtle and complicated features of the fracture geometry, such as the size of connected clusters, the size of unfractured blocks (Figures 3 and 4) and the "shape factor" which is often used in dual-porosity flow simulators to capture the fracture-matrix connectivity.

Figure 3. **The size of unfractured blocks on Lägerdorf Wall #11, as calculated from the actual mapped fractures (top), and from two simulations (bottom) of the 3-D fracture network model sliced along the plane corresponding to Wall #11. The grey circles mark unfractured regions that are locally maximal in extent.**

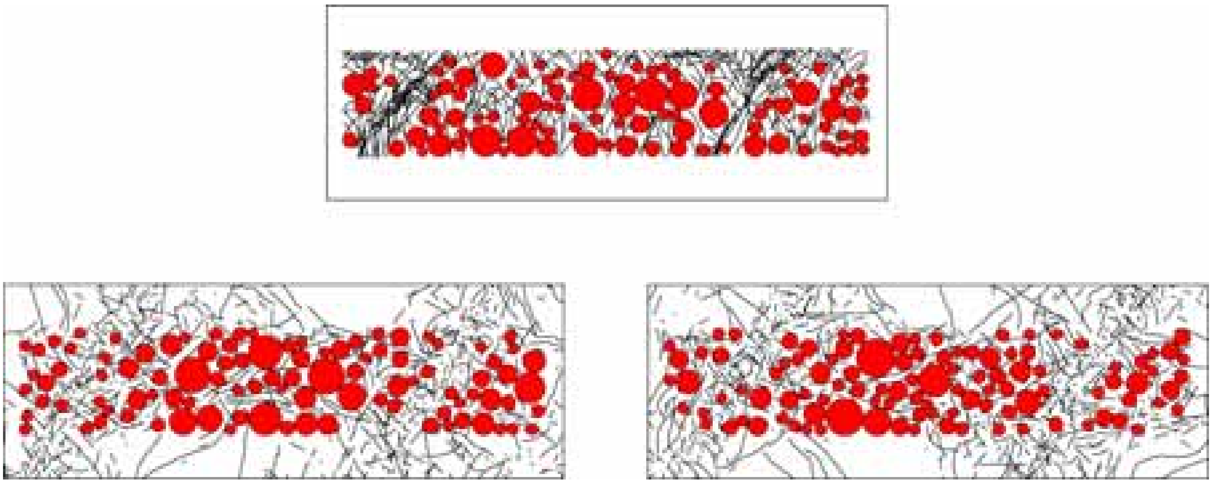
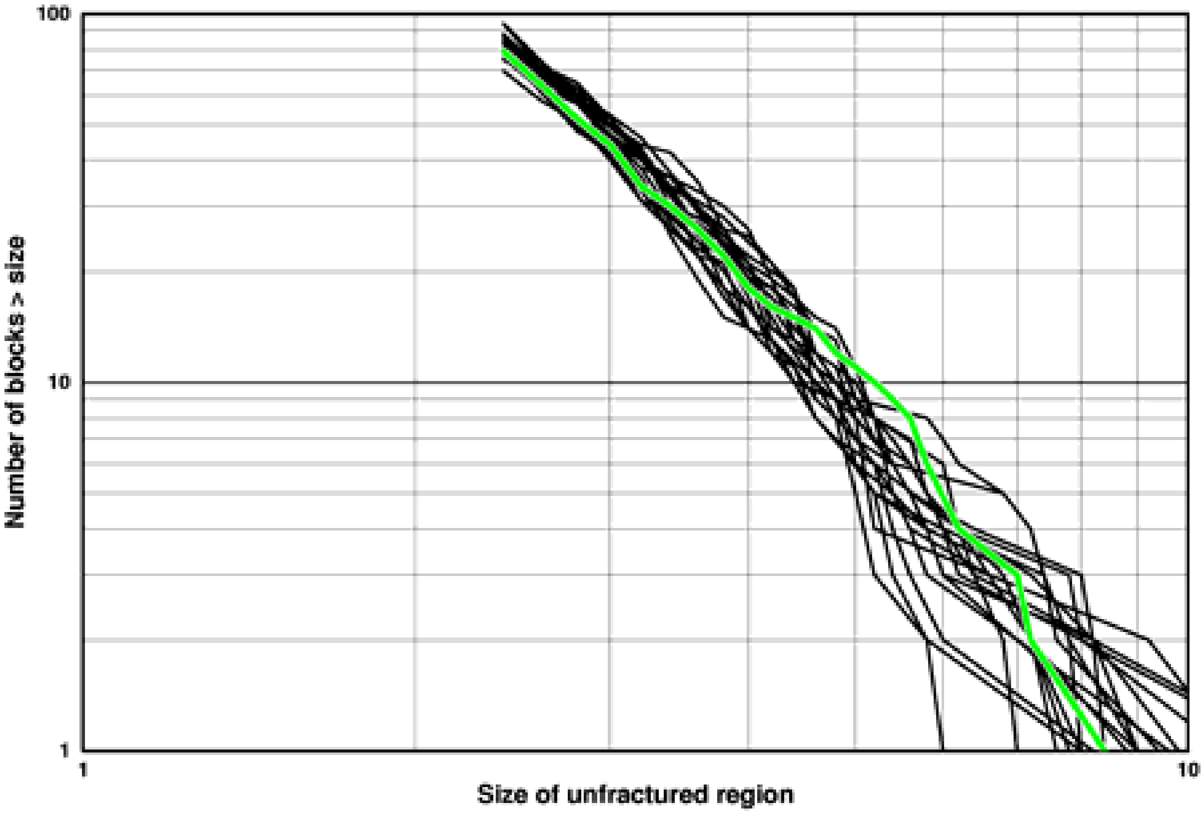


Figure 4. **The cumulative size distribution of unfractured regions from 20 simulations (black lines) versus the actual data from Lägerdorf Wall #11 (grey line).**



4. Summary and conclusions

By accommodating all of the these various pieces of "hard" and "soft" data, these FNMs provide a single, coherent and consistent model that can serve the needs of many preliminary site characterisation studies. The detailed, complex and realistic models of 3-D fracture geometry produced by this method can serve as the basis for developing rock property models to be used in flow and transport studies. They can also be used for exploring the suitability of a proposed site by providing quantitative assessments of the probability that a proposed repository with a specified geometry will be intersected by fractures. When integrated with state-of-the-art scientific visualisation, these models can also help in the planning of additional data gathering activities by identifying critical fractures that merit further detailed investigation. Finally, these FNMs can serve as one of the central elements of the presentation and explanation of the Descriptive Conceptual Geosphere Model (DCM) to other interested parties, including non-technical audiences.

In addition to being ideally suited to preliminary site characterisation, the approach also readily incorporates field data that may become available during subsequent site investigations, including ground reconnaissance, borehole programmes and other subsurface studies. A single approach can therefore serve the needs of the site characterisation from its inception through several years of data collection and more detailed site-specific investigations, accommodating new data as they become available and updating the FNMs accordingly.

The FNMs from this method are probabilistic in the sense that they consist of a family of equally likely renditions of fracture geometry, each one honouring the same surface and subsurface constraints. Such probabilistic models are well suited to studying issues involving risk assessment and quantification of uncertainty. This assists the exploration of geoscientific uncertainty and how the inherent non-uniqueness of DCMs affects confidence in predictions of how the far-field geosphere affects overall safety of the proposed repository.

The approach provides models that are systematic and traceable in the sense that all of the data, assumptions and parameter choices are clearly recorded and auditable. At the same time that subjective decisions are avoided, the various parameter choices still allow reasoned judgement from structural geology and geomechanics to constrain the model. By providing placeholders for such judgements, this approach moves this type of information from an undocumented constraint to a reviewable parameter choice.

The technical consistency of these FNMs, their auditability and their visual and scientific realism all contribute to the presentation of geologic safety arguments that demonstrate good judgement, thereby increasing confidence in the entire modelling effort.

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THE EVOLUTION OF GROUNDWATER FLOW AND MASS TRANSPORT IN CANADIAN SHIELD FLOW DOMAINS: A METHODOLOGY FOR NUMERICAL SIMULATION

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1. Introduction

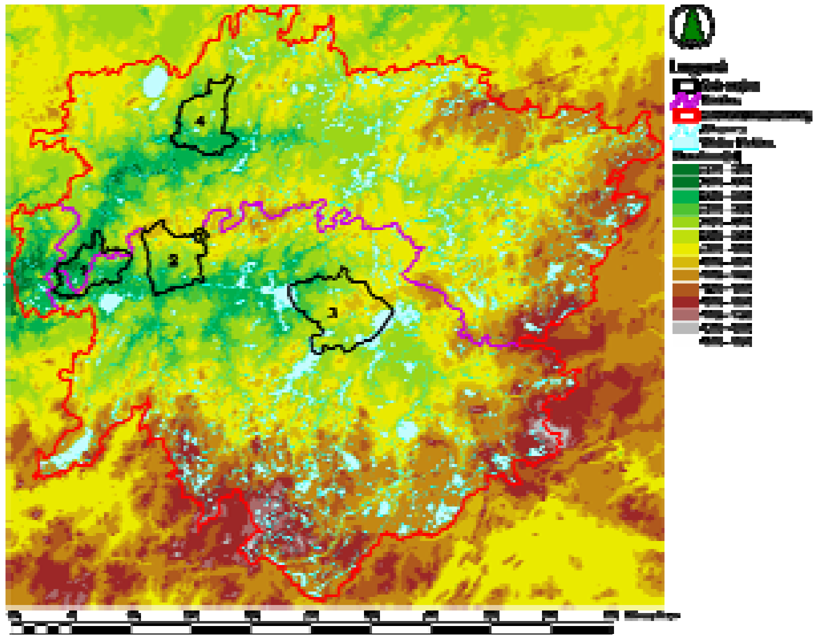
The Deep Geologic Repository Technology Programme (DGRTP) of Ontario Power Generation (OPG) is exploring methods to advance the application of numerical methods for the simulation and prediction of groundwater flow and mass transport in crystalline Shield settings. The intent is to illustrate numerical methods and modelling approaches capable of aiding site characterisation in the iterative and multi-disciplinary derivation of descriptive conceptual geosphere site models. A key aspect of this work is associated with developing methods to improve field data traceability within numerical simulations of heterogeneous and anisotropic flow domains, particularly those influenced by fracture zone networks. This approach is intent on providing a systematic framework with which to assemble complex spatial and temporal geoscientific data sets and conduct quantitative flow system uncertainty analyses.

The potential suitability of a candidate site to host a geologic repository will rely, in part, on a demonstrated understanding of the groundwater flow system and its evolution over time scales of perhaps tens of thousands of years or greater. The characterisation of a flow system is achieved through an iterative site characterisation process in which multi-disciplinary lithostructural; hydrogeologic, paleohydrogeologic, geophysical, hydrogeochemical and geomechanical data are gathered at increasing levels of detail to support development of a conceptual flow system model. At each successive stage of this iterative process, data are used to query and test the existing conceptual flow system model and make modifications as necessary. Numerical flow system analyses offer a systematic framework in which these site specific data may be integrated and then assessed for consistency. Such Performance Assessment or Site Characterisation analyses can instill confidence in the conceptual flow system model(s) and provide a basis for predictive modelling of long-term flow system evolution and repository performance.

This extended abstract, describes work undertaken for Ontario Power Generation's Deep Geologic Repository Technology Programme (DGRTP). The first phase of the work programme involved an illustrative numerical analysis of groundwater flow in a hypothetical Shield-like regional flow domain (refer to Figure 1). Principal concerns are the evolution and distribution of physical and chemical flow system properties on regional groundwater characteristics. Another issue is that of long-term climate change (e.g. impacts of continental-scale glaciation) and the influence of time-dependent hydraulic and mechanical boundary conditions on flow system evolution at time scales relevant to repository safety.

The second phase of the work investigated sub-regional and repository scale groundwater flow in a fractured crystalline rock setting characteristic of the Canadian Shield. The sub-regional analysis was performed using a portion (area 2 shown in Figure 1) of the hypothetical regional flow domain, but at a much higher computational resolution. Parameters and characteristics for the regional and sub-regional domain were derived, in part, from data gathered at geoscience research areas under study during the Canadian Nuclear Fuel Waste Management Programme, such as the Underground Research Laboratory located at Lac du Bonnet in the province of Manitoba, Canada. Data from other crystalline rock settings, including published information gathered from Finland and Sweden, were also incorporated in our analyses.

Figure 1. **Regional scale domain showing DEM, surface water features and selected sub-regional domains.**



The third phase of the work programme included an evaluation of the numerical models SWIFT-III and FRAC3DVS that were used for the three-dimensional regional and sub-regional analyses. Uncertainty analyses were also undertaken, with the stochastic parameters including equally probable fracture network models (including the impact of conditioning *via* their surface expressions), fracture permeability and thickness, and the depth-dependent permeability of the moderately- and sparsely-fractured host rock. The performance measure developed for the uncertainty analysis included groundwater age. In our ongoing work, the impact of an evolving glacial climate, including the effects of glacial ice loading, permafrost formation/melting and high-salinity brines located at depth in the Shield, on the transient groundwater flow regime is being assessed.

2. Regional scale analyses

A three-dimensional numerical analysis of a hypothetical 5 734 km^2 watershed situated on the Canadian Shield in the Superior Province was conducted to illustrate aspects of regional scale groundwater flow within a typical Shield setting. An essential requirement for analysis of regional scale groundwater flow in a crystalline Shield setting was the preservation and accurate description of the complex topography and surface water drainage network characteristic of such systems. The description must also represent the groundwater salinity and permeability distributions, particularly with depth. To include the attributes of the complex surface topography in the conceptual model of the watershed, ArcView GIS and Visual Basic pre-processors were used for data management and manipulation. These tools facilitated the development of a discretised model domain with 1 534 080 finite difference grid blocks. Domains with over 6 million grid blocks also have been developed. Digital input data for the conceptual model included a digital elevation model (DEM), a bedrock geology map, a Quaternary geology map and a water features map that defined rivers, lakes and wetlands. Simplifying and possibly conflicting assumptions associated with abstracted models having reduced physical dimensionality are not necessary as the three-dimensional nature of the topography, surface water features, and the spatial variation of the rock permeability values have all been natively incorporated within the model framework.

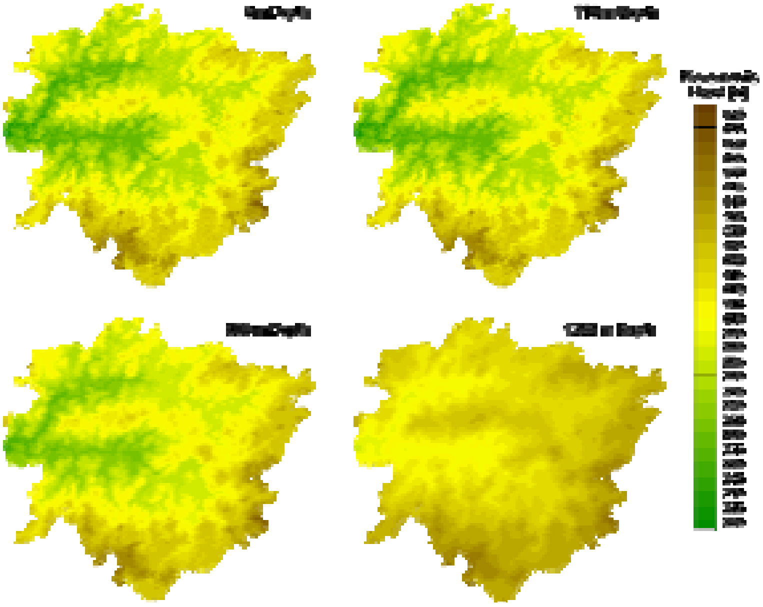
At the regional scale, the post-glacial evolution of the groundwater flow system was investigated using the Equivalent Porous Medium (EPM) finite difference model SWIFT-III in which the fluid density and viscosity are fully dependent on the fluid pressure, temperature and groundwater salinity. The model domain, which extends 102 km in the east-to-west direction and 94 km in the north-to-south direction, was discretised to a depth of 1.5 km using 10 layers. The robustness of the groundwater flow system was assessed by exploring the sensitivity of groundwater flow to topography, variable rock permeability-depth distribution models, pore water salinity and the rate of dissipation of elevated paleo-pore-pressures that resulted from ice that overlaid the watershed over the last glacial period.

Steady-state groundwater flow analyses indicate that piezometric heads in all model layers are highly correlated to the complex surface topography (refer to Figure 2). The complexity results in the transition from zones of groundwater recharge to discharge over distances that can be relatively short. This variation, coupled with rock permeability values that decrease significantly with depth, results in a groundwater system where shallow flow to a depth of tens of meters dominates the overall water balance and the length of flow paths is relatively short. The flow that occurs in the deeper rock, for example at depths greater than 700 m, represents a small fraction of the total water budget in the context of the entire watershed. The analyses evolving from this study indicate that the flow in this deeper rock regime is not regional but rather is a subdued reflection of the local-scale surface topography. For the hypothetical watershed investigated in this study, groundwater was not predicted to underflow the major rivers and their tributaries.

A series of transient analyses provided evidence that for horizons greater than 600 m in depth, the low permeability (10^{-19}-10^{-17} m^2) of the granitic rock, coupled with saline pore water, creates a sluggish flow system in which mass transport appears to be diffusion dominated. The sluggish movement of denser pore waters due to salinity has a profound effect on the travel times of average water particle paths and induces density gradients that can enhance or reduce topographically driven gradients.

Field evidence indicates that the sparsely fractured rock in the Canadian Shield may contain highly saline porewaters at pressures that may be higher than can be explained by current surface topography. Transient groundwater models that fully couple flow, glacial loading and salinity transport are therefore required to analyse both the impact of the salinity on the groundwater flow system and the dissipation of the glacially-induced over-pressurised paleo impacts for these evolving systems. Shown in Figure 3 are the total dissolved solids concentrations in a selected cross-section of the three-dimensional regional domain at 100 000 years. Our analyses clearly indicate that steady-state cross-sectional models cannot be used to capture the relevant 3-D flow and transport processes. The preservation of elevated pressures at depth in the rock after 10 000 years from an initial elevated hydrostatic state imposed by glacial loading requires the use of a depth-hydraulic conductivity for the rock such that

Figure 2. **Piezometric heads at various depths at 10 000 years for base case regional analysis and fresh water in all model layers.**



the inferred trend declines to a value less than about than 2.23 × 10^{-11}m/s at depths greater than about 800 m. In essence, our computational framework and methods of analyses are intended to preserve the salient features associated with the complexity of the watershed-scale groundwater system, with a concomitant enhancement of computational algorithms to enhance repository performance assessment using minimal model abstraction.

3. Sub-regional scale analyses

The objective of this phase of the DGRTP work programme was to advance the integration and application of data management, numerical methods, visualisation and safety assessment for the analysis of sub-regional crystalline plutonic flow systems. A key element of the work was the use of the numerical model FRAC3DVS for the solution of three-dimensional variably-saturated groundwater flow and solute transport problem in porous and discretely-fractured media. The model allows the inclusion of discrete features such as complex-structured curvilinear fractures. In a crystalline rock setting, these fractures are believed to be comprised of zones of higher permeability within the moderately- and sparsely-fractured bulk rock. Using FRAC3DVS, flow and transport in the fracture zones are approximated using an equivalent porous medium formulation, but treating the fracture zones to have enhanced flow and dispersive properties compared to those of the host rock. The numerical solution to the governing nonlinear, coupled flow and transport equations is based on implementations of either the finite-volume or the Galerkin finite-element method. Both steady-state and transient analyses were undertaken with the objective of the former being the investigation of the spatial properties of the sub-regional conceptual model.

Figure 3. **Salinity concentrations – cross-section at 100 000 yr; case 2 (2.23 x 10^{-13} m/s below 700 m) with 1.03 g/cm^3 density.**

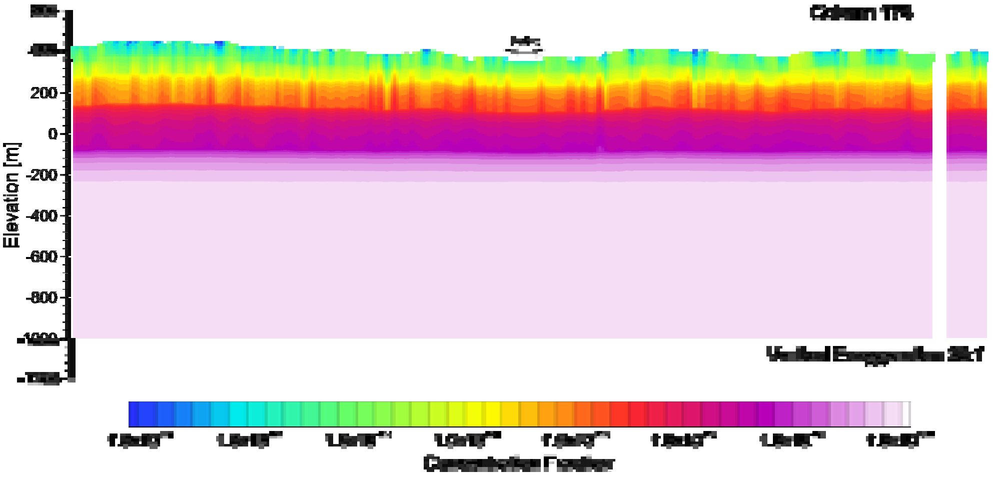
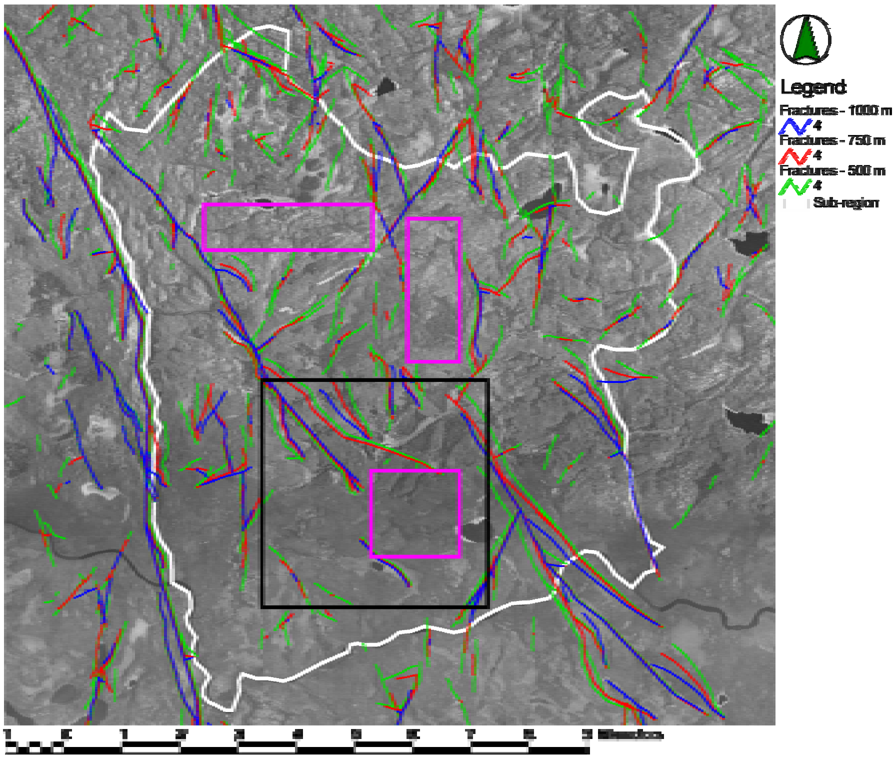
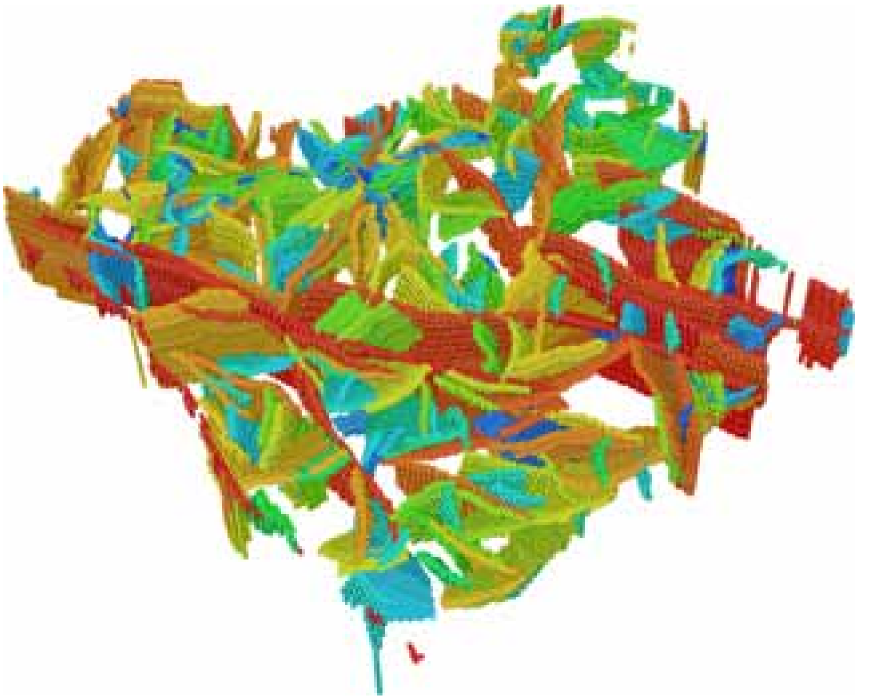


Figure 4. **Sub-region 2 showing aerial photo, surface water features, and fracture intersections at various depths. Possible repository locations (purple rectangles of 2.25 km^2) and possible site perimeter (black square of 15 km^2) are also shown.**



Transient analyses were required for both the simulation of flow with coupled pressure, concentration and temperature and the simulation of the impact of future glaciation. A detailed groundwater flow analysis of an 84 km^2 portion of the regional 5 734 km^2 watershed in a hypothetical Canadian Shield setting was conducted to illustrate aspects of regional and sub-regional groundwater flow relevant to the long-term performance of a hypothetical nuclear fuel repository. FRAC3DVS was used to investigate the importance of large-scale fracture networks on flow and advective particle migration. Surface water features and a Digital Elevation Model (DEM) were applied in a GIS framework to delineate the sub-watershed and to populate the finite element mesh. The boundary conditions for the domain are derived from the regional groundwater flow system. As part of the analysis, a complex geostatistically derived three-dimensional probabilistic Fracture Network Model (FNM) was superimposed onto a 600 000 element flow domain mesh. Orthogonal fracture faces (between adjacent finite element blocks) were used to best represent the irregular FNM. Figure 4 shows the fracture intersections at various depths for a single realisation of the FNM while a perspective plot of the discretised FNM is shown in Figure 5. The crystalline rock mass between these structural discontinuities was assigned a range of properties considered characteristic of Shield terrain. Interconnectivity of permeable discontinuities, particularly at depth, is required to create discrete pathways for relatively rapid migration of average water particles and subsequent reduction in residence times.

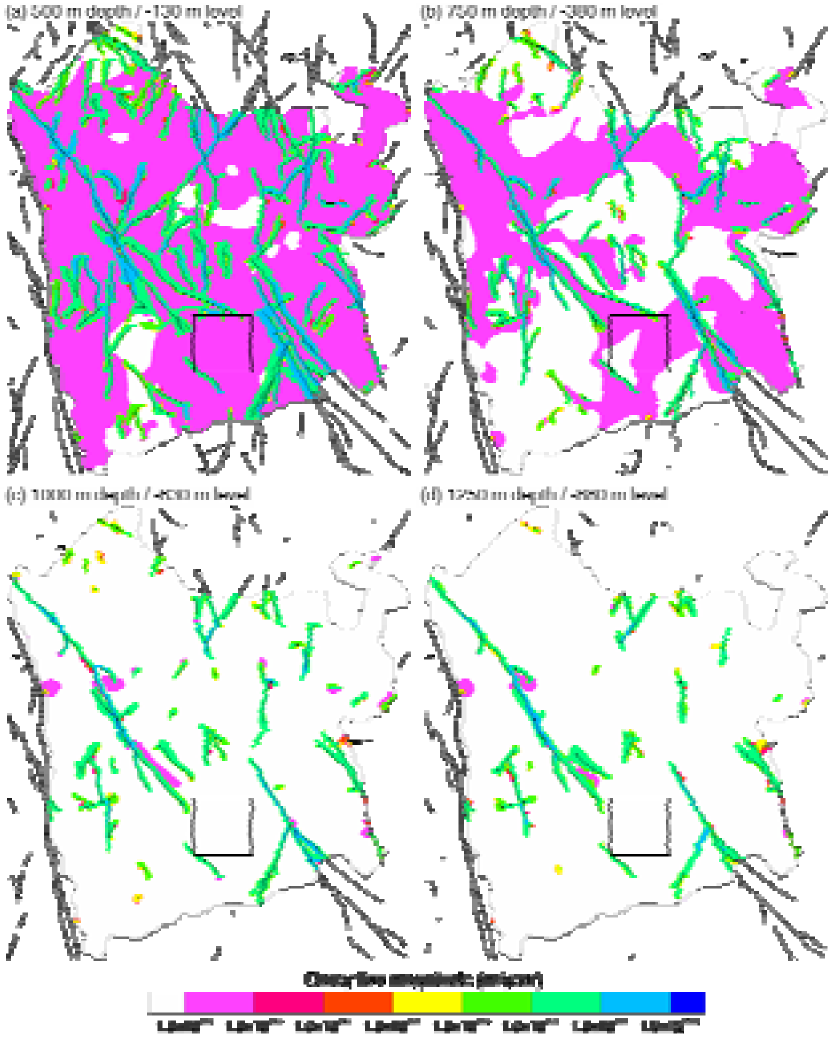
Figure 5. **3-D perspective view of the FRAC3DVS fractures.**



The use of realistic topography, delineation of fracture zone networks that honour many geological, statistical, and geomechanical constraints, and the use of fine discretisation grids have improved upon the previous studies of a similar nature. From the analyses, predicted Darcy fluxes at depths below approximately 600 m are indicative of mass transport regimes in which diffusion would be the dominant transport mechanism (refer to Figure 6).

This work has provided new insights into the behaviour of flow systems in a Shield-like environment that contains a topologically complex network of fracture zones. The findings are intent on developing a better understanding of flow system evolution at sub-regional watershed scales, particularly as affected by long-term climate change, and to assess the robustness of numerical predictions given site-specific characterisation uncertainty.

Figure 6. **Case 1 Darcy flux magnitudes and the corresponding intersecting fractures at various depths.**



4. FRAC3DVS and SWIFT-III verification

In the verification study, groundwater flow and transport modelling results simulated using the numerical models SWIFT-III and FRAC3DVS were compared for the regional (5 734 km^2) watershed. For the purposes of the verification study, nine of the sixteen flow domain scenarios modeled using SWIFT-III were chosen for comparison with FRAC3DVS. These scenarios involved consideration of increasing flow system complexity ranging from fresh, homogeneous and steady-state conditions to saline, heterogeneous and transient conditions. The results of the study revealed not only a favourable comparison between the predicted results obtained with both models for the simulated test cases, but also revealed areas in which code performance for application to deep-seated regional flow systems in fractured rock can be improved.

To make code comparison more precise, the finite difference and finite element grids for the two models were purposely meshed such that calculational points were coincident. This required that the FRAC3DVS finite element blocks be offset by one-half a grid element as compared to the

SWIFT-III finite difference grid. The number of layers in FRAC3DVS was doubled as compared to SWIFT-III in order to ensure that the vertically variable hydraulic conductivity would coincide spatially in both models.

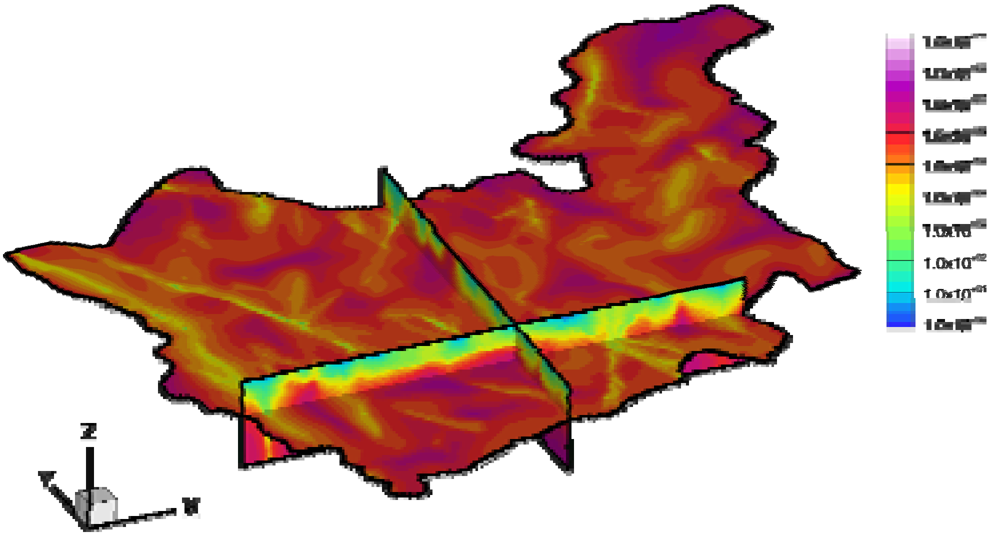
For the purpose of comparison, estimated model values such as piezometric head or pressure at datum, Darcy velocity and fractional (or relative) concentration were chosen as performance measures. Although the piezometric heads or pressures at datum, and relative concentration could be directly compared at calculational points, excess surface infiltration along the perimeter of the SWIFT-III realisations due to horizontal discretisation was evident in comparison to the FRAC3DVS results. Spatially, the correlated hydraulic conductivity values could not be made precisely coincident given grid block offsets. Despite these issues, the model results are shown to compare well with reasoned explanations. Based on the results of this study, FRAC3DVS does have notable advantages over SWIFT-III.

5. Uncertainty analysis, the life expectancy performance measure and glacial evolution

The Sub-regional Groundwater Flow System Case study involved a detailed flow analysis of an 84 km^2 portion of the regional Shield watershed. This sub-regional flow system case study provided valuable insight into the behaviour of flow domains containing complex, 3-dimensional, curvilinear fracture zones; however, a number of modelling scenarios relevant to a deep geologic repository and the impact of long-term climate change were considered a logical extension of the programme. These additional scenarios would: i) incorporate two cases involving multiple stochastic realisations (up to 100) of the fracture network model, with the first case constrained to preserve the measured surface lineaments supplemented by a single realisation of the remaining generated or infilled lineaments, and a second case where there are many stochastic realisations of the infilled lineaments; ii) investigate the role of variable-density groundwaters (salinity); iii) explore the impact of more realistic, spatially-correlated, permeability fields in the fracture zones and the rock matrix continua; and iv) include transient analyses governed by the time history of pore pressure dissipation associated with glacial cycles. The fourth modelling scenario is developed from the simulation of climate-driven Laurentide glacial ice-sheet history, including the influence of permafrost. The transient analysis includes the development of a permafrost layer and the evolution of the surface boundary conditions in response to glaciation.

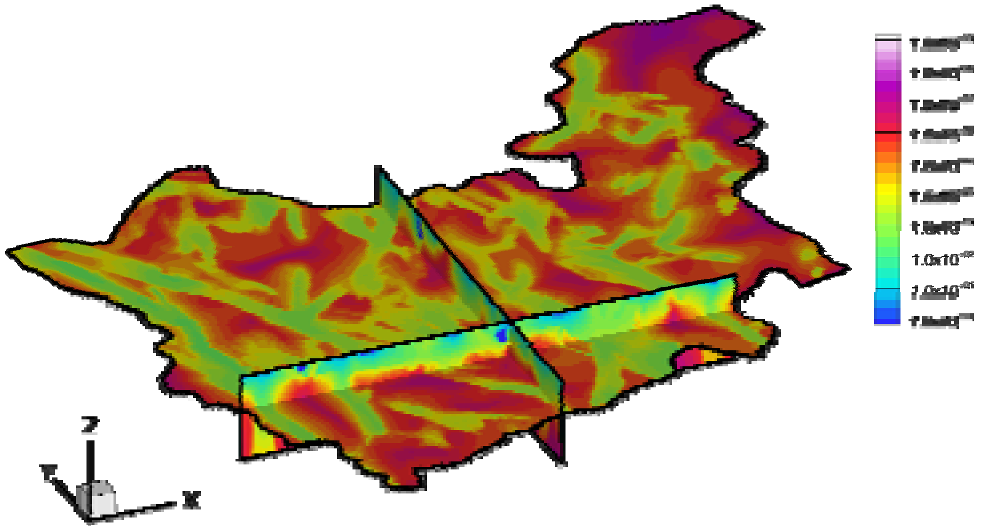
All work was integrated with the MIRARCO Virtual Reality Technology Programme for multi-disciplinary data integration and communication of the sub-regional conceptual geosphere model database and simulation results. The goal in undertaking these modelling activities was to illustrate and visualise the flow system and to assess whether it remains stagnant and diffusion-dominated at repository depths regardless of the uncertainty in the fracture zone geometry and interconnectivity. Further, the issue of whether glacial, oxygenated waters could migrate to depths as a result of the significant changes in surface boundary conditions associated with future and past glaciation events was addressed.

Figure 7. **Sub-regional scale estimation of life expectancy (years) for 100 realisations of fracture geometry conditioned to surface lineaments: (a) 50th percentile of life expectancy.**



(b) 5th percentile of life expectancy

(a)



(b)

The evaluation of uncertain radionuclide travel times from a repository to the biosphere is critically important in a performance assessment analysis. For this work, a travel time framework based on the concept of groundwater lifetime expectancy as a safety indicator was developed. Lifetime expectancy characterises the time radionuclides will spend in the subsurface after their release from the repository and prior to discharging into the biosphere. The probability density function of lifetime expectancy is computed throughout the host rock by solving the backward-in-time solute transport equation subject to a properly posed set of boundary conditions. It can then be used to define optimal repository locations. Figure 7 presents the life expectancy for the sub-regional analysis with the 50th and 5th percentile values being plotted from 100 Monte Carlo realisations of the FNM conditioned on the surface lineaments. The 5th percentile represents a 5% chance that travel times are less than those shown in Figure 7b. In a second step, the risk associated with selected sites can be evaluated by simulating an appropriate contaminant release history. Based on a statistically-generated three-dimension network of fracture zones embedded in the granitic host rock, the sensitivity and the uncertainty of lifetime expectancy to the hydraulic and dispersive properties of the fracture network, including the impact of conditioning via their surface expressions, is computed.

6. Summary

The Deep Geologic Repository Technology Programme (DGRTP) of Ontario Power Generation (OPG) is developing numerous approaches and methodologies for integrated and multidisciplinary site characterisation. A principal element involves the use and further development of state-of-the-art numerical simulators, and immersive visualisation technologies, while fully honouring multi-disciplinary lithostructural, hydrogeologic, paleohydrogeologic, geophysical, hydrogeochemical and geomechanical field data.

Paleo-climate reconstructions provide surface boundary conditions for numerical models of the subsurface, furthering the understanding of groundwater flow in deep geologic systems and quantifying the effects of glaciation and deglaciation events. The use of geostatistically plausible fracture networks conditioned on surface lineaments within the numerical models results in more physically representative and realistic characterisations of the repository site.

Finally, immersive three-dimensional visualisation technology is used to query, investigate, explore and understand both the raw data, and simulation results in a spatially and temporally consistent framework. This environment allows multi-disciplinary teams of geoscience professionals to explore each other’s work and can significantly enhance understanding and knowledge, thereby creating stronger linkages between the geoscientific disciplines. The use of more physically representative and realistic conceptual models, coupled with immersive visualisation, contributes to an overall integrated approach to site characterisation, instilling further confidence in the understanding of flow system evolution.

GEOSCIENTIFIC INFORMATION IN THE ASSESSMENT OF LONG TERM SAFETY: APPLICATION OF CNSC REGULATORY GUIDE G-320

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The Canadian Nuclear Safety Commission (CNSC) regulates the nuclear industry in Canada under the authority of the *Nuclear Safety and Control Act* (1997) [1]. This Act prohibits numerous activities related to the use of nuclear energy and nuclear substances unless those activities are licensed by the CNSC. Amongst the prohibitions, a person or organisation needs a licence to possess, mine, refine, manage, store or dispose of a nuclear substance, or to prepare a site, construct, operate, modify, decommission or abandon a nuclear facility.

The mandate given to the CNSC by the Act includes regulation of the development, production and use of nuclear energy in Canada and regulation of the production, possession, use and transport of nuclear substances, in order to prevent unreasonable risk to the health and safety of persons, to the environment and to national security.

1. Regulatory structure

The CNSC fulfills its mandate through a comprehensive cradle-to-grave licensing system. This system includes critical assessment of licence applications to determine the safety of the proposed activities and the qualifications of the applicant, a comprehensive compliance verification programme and a graduated enforcement programme (enforcement commensurate with the infraction). The approach adopted by the CNSC to achieve its objectives is non-prescriptive. Applicants are free to propose their preferred approach to meeting the regulatory requirements, and then they must convince the CNSC that they can make their proposed approach work.

The CNSC is composed of two independent parts: the Commission and CNSC Staff. The Commission is a quasi-judicial tribunal, appointed by the Government, with the authority to issue licences. CNSC staff makes recommendations to the Commission on licence applications, and then administers the licences once they are issued.

The licensing process includes CNSC staff assessment of a licence application, to determine the safety of the proposed activities. Before placing the licence application and its recommendation before the Commission in a public hearing, CNSC Staff must be satisfied that the application meets the requirements set out in the Act and Regulations pursuant to the Act, that the activities to be licensed will be safe, and that the applicant is qualified to carry out those activities.

Staff recommendations cannot, and do not, bind the Commission. During the public hearings, the Commission can interrogate the applicant to clarify or add to the information submitted in the licence application. The Commission also questions CNSC Staff regarding the basis for its recommendation. Hence, CNSC Staff has to defend its recommendation. This means that Staff must be convinced of the safety of the activities to be licensed. The Staff review is often critical of a licence application, demanding corrections and revisions until Staff is satisfied its recommendation is defensible.

2. Regulating radioactive waste

A licence application must contain information to demonstrate that the regulatory requirements will be met. The regulatory requirements with which licensees must legally comply are set down in statutory instruments such as legislation, regulations and licences. The *Nuclear Safety and Control Act* not only gives the CNSC its authority, it specifies generic regulatory requirements. The set of nine regulations pursuant to the Act[1] define more specific requirements and information needs. Individual case-by-case requirements can be specified as conditions in a licence.

The CNSC also makes use of non-statutory instruments such as Regulatory Policies, Regulatory Standards, Regulatory Guides and Regulatory Notices. Regulatory Policies describe the philosophy, principles or fundamental factors that underlie the CNSC's approach to its regulatory mission. For example, Regulatory Policy P-290, Managing Radioactive Wastes [2], establishes that radioactive waste is subject to the Act and regulations and sets out the CNSC expectations for the safe management of waste facility operations and expectations of long term protection from the hazards of the waste.

Regulatory Guides indicate acceptable ways of meeting, within the framework of Regulatory Policies, the regulatory requirements expressed in the Act, regulations and licences. Building on the principles expressed in P-290, Regulatory Guide G-320, Assessing the Long-term Safety of Radioactive Waste Management [3], provides generic guidance on how to assess the safety of waste management systems for the long term and what the CNSC expects to be included in such assessments. G-320 applies to any assessment of the long term safety of all types of radioactive waste – whether the waste is from the nuclear fuel cycle, research, medical and industrial applications or historic waste.

3. Assessing long-term safety

A licence applicant should provide reasonable assurance that the regulatory requirements for long term safety and protection can be met. G-320 provides guidance on steps that are commonly considered in safety assessments, such as assessment methodology and approach, safety criteria, defining critical groups and scenarios, time frames, confidence in assessment findings and the use of institutional controls. The guide provides a basis for case-by-case discussions with licence applicants on more focused guidance that takes into consideration the applicant's particular circumstances.

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[1] The regulations pursuant to the Nuclear Safety and Control Act are:

- General Nuclear Safety and Control Regulations.
- Radiation Protection Regulations.
- Class I Nuclear Facilities Regulations.
- Class II Nuclear Facilities and Prescribed Equipment Regulations.
- Uranium Mines and Mills Regulations.
- Nuclear Substance and Radiation Devices Regulations.
- Packaging and Transport of Nuclear Substance Regulations.
- Nuclear Security Regulations.
- Nuclear Non-proliferation Import and Export Control Regulations.

These regulations and the Nuclear Safety and Control Act are accessible on the Regulatory & Licensing Information page on the CNSC website at www.nuclearsafety.gc.ca.

The information required in a licence application defines the need for long term assessments. Licence applications require, among other things:

- information about effects on the environment and the health and safety of persons that may result from the activities that are to be licensed;
- information to enable the Commission to determine whether adequate provision will be made to protect the environment; and
- an assessment of the potential environmental effects of the proposed decommissioning programme that must be included in the application.

Long term assessment of safety of waste management systems plays an important role in designing a facility, evaluating its possible environmental impacts, preparing decommissioning plans and in establishing a safety case for licence approval and public acceptance. A broad range of assessment approach, level of detail and degree of rigor is possible, based on the available information and on the purpose intended for the assessment results.

Prior to licensing, safety assessments can be used in site selection and in optimising the facility design. The CNSC expects the design of a facility to have been optimised to more than just meet the regulatory limits. The waste management system should be optimised so that its predicted impacts remain below the regulatory limits by some margin of safety. In addition, a long term assessment is an integral part of an Environmental Assessment of waste management facilities, which may be required under the Canadian Environmental Assessment Act before the CNSC can exercise its regulatory authority.

G-320 recognises the distinction between a safety assessment and a safety case. The collection of supporting arguments that is included in the safety case to substantiate and provide confidence in the results of the safety assessment provides increased assurance of long-term safety. G-320 discusses the need for a clear presentation of the supporting arguments and how they fit together in the safety case.

G-320 also discusses the development of the scenarios for safety assessments. These scenarios should be based on receptor characteristics, waste properties and site characteristics. The scenarios may include a base case scenario of expected conditions and normal evolution of the site for the safety assessment, and additional scenarios whose analysis provides supporting arguments for the safety case, such as:

- extreme conditions or disruptive events;
- unexpected containment failure (including human intrusion);
- limiting and bounding conditions; and
- natural analogs that are similar to the waste management system being evaluated.

Since uncertainties increase with longer time frames of assessment, the results of long term predictions should only be considered to be indicators that compliance with current regulatory requirements for protection will continue into the future. G-320 discusses approaches for incorporating a margin of safety in the assessment, to compensate for the uncertainty in making long term predictions, the uncertainty in future human actions and the possibility that the waste management system may not be the only source of contaminants to which the receptor is exposed.

A margin of safety can be demonstrated by comparing conservative (or over-estimate) calculations to the regulatory limits, or by comparing 'best estimate' calculations to a design target which is some fraction of the regulatory limit. Either of these approaches should provide reasonable assurance of the long term safety.

4. Using geoscientific information

Geoscientific information is needed to develop a site descriptive model, which can then be used in site selection, in facility design, and in developing plans for decommissioning. Geoscientific information provides pre-construction baseline data for a site, and provides background conditions from monitoring reference sites. Such information needed to be able to differentiate between undisturbed conditions and facility-related effects.

A safety assessment also makes use of geoscientific information, to identify Features, Events and Processes (FEPs) that go into developing the scenarios that are analysed. These scenarios can include the expected evolution of the site, extreme conditions that the site could be subjected to, and the type, frequency and magnitude of disruptive events that could occur. The geoscientific information used in scenario development may vary from generic default data to site-specific characterisation data.

In addition to assessments of a suite of scenarios, reasoned arguments can be used in support of a safety case. These supporting arguments can be based on complementary safety indicators which are derived from analysis of the geoscientific information. These analyses can include the paleo-history of the site, models of concurrent independent geochemical systems, natural analogs of processes expected to occur in the waste management facility, and response of the site to construction, operation and extreme conditions or disruptive events based on analysis of the site's response to perturbations during its evolutionary history.

Geoscientific information is usually collected using a site characterisation plan that is implemented before the licensing process is initiated by an application to the CNSC. Hence, a site characterisation plan does not need regulatory approval, and some important geoscientific information can be collected without regulatory oversight. However, Regulatory Guide G-320 identifies the CNSC's expectations that the geoscientific information, from which a conceptual site model will be derived and which will figure prominently in the designing a facility, will be collected, managed and interpreted under formal quality assurance and quality control (QA/QC) protocols. This reflects the need for the information underlying the licence application to be retrievable, auditable and defensible.

The diversity and breadth of geoscientific information and the wide array of the ways it can be used invoke the need for careful management of the knowledge and clear presentation of the information and the way it is used. Designing a site investigation programme to acquire, manage and use the extensive range of geoscientific information will be a key element in successfully characterising a site (meaning that the right information is collected in a usable manner). Careful planning is needed, which could begin with identifying the end use of the information and then working backwards through the reasoned arguments that will be prepared and the interpretation techniques that will be used, to finally arrive at identifying the site characteristics and properties that need to be measured. This is similar in concept to inverse modelling or reverse engineering of the process of site characterisation, safety assessment analysis, safety case preparation and decision making. The plan, then, guides not only the site characterisation activities, but also how that information is used to support the safety case.

Presentation of the large number of reasoned arguments that can be used in a safety case can be confusing. There is a need for a clear "roadmap", a statement of structure of the safety case and repeated identification of where and how each argument fits in. This is to help prevent readers of the safety case from focusing inappropriate or misdirected attention on an individual supporting argument or on uncertainties in underlying geoscientific information and interpretation, instead of considering the overall weight of evidence of the safety case.

The geoscientific information, its interpretation and the Safety Case arguments should be presented in a manner that prevents raising concerns about: how representative are individual measurements; how accurate is the up-scaling from measurement scale to site scale; how appropriate is the inductive reasoning process that infers site-wide characteristics from specific measurements; have the measurements provided the data the safety assessment models need; and are model simplifications (such as an equivalent porous medium interpolation) adequate to represent the site descriptive model.

There can be other concerns related to how individual safety assessments and other supporting arguments are used within the safety case, such as: are arguments that are given equal weight in the safety case developed with equal level of detail and rigor; is the uncertainty in important supporting arguments ignored in favour of improving confidence in another supporting argument that is less important; and are some of the arguments founded on expert opinion that is not recognised and qualified in the presentation of the argument.

The issues about geoscientific information, its use and presentation are among the issues addressed in Regulatory Guide G-320. The guide was prepared after a pre-consultation with the major producers and owners of radioactive waste to identify the issues on which they need guidance. Not all of the guidance offered in G-320 will be applicable to every assessment of long term safety, as the guidance is designed to be useful for a broad range of assessment approaches. Where the guidance is not specific, it is expected that the applicant will engage in discussions with the CNSC to obtain case-specific guidance appropriate for the circumstances of their site, facility design and safety case methodology.

References

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[2] Regulatory Policy P-290, Managing Radioactive Wastes, Canadian Nuclear Safety Commission, Ottawa, 2004. www.nuclearsafety.gc.ca/pubs_catalogue/uploads/P290_e.pdf }.

[3] Regulatory Guide G-320, Assessing the Long Term Safety of Radioactive Waste Management (Draft), Canadian Nuclear Safety Commission, Ottawa, 2005. www.nuclearsafety.gc.ca/pubs_catalogue/uploads/G-320PublicConsultationApril05_e.pdf.

POTENTIALS AND LIMITATIONS OF THE USE OF GEOHISTORY FOR THE UNDERSTANDING OF CURRENT FEATURES AND CONDITIONS AND POSSIBLE FUTURE EVOLUTIONS

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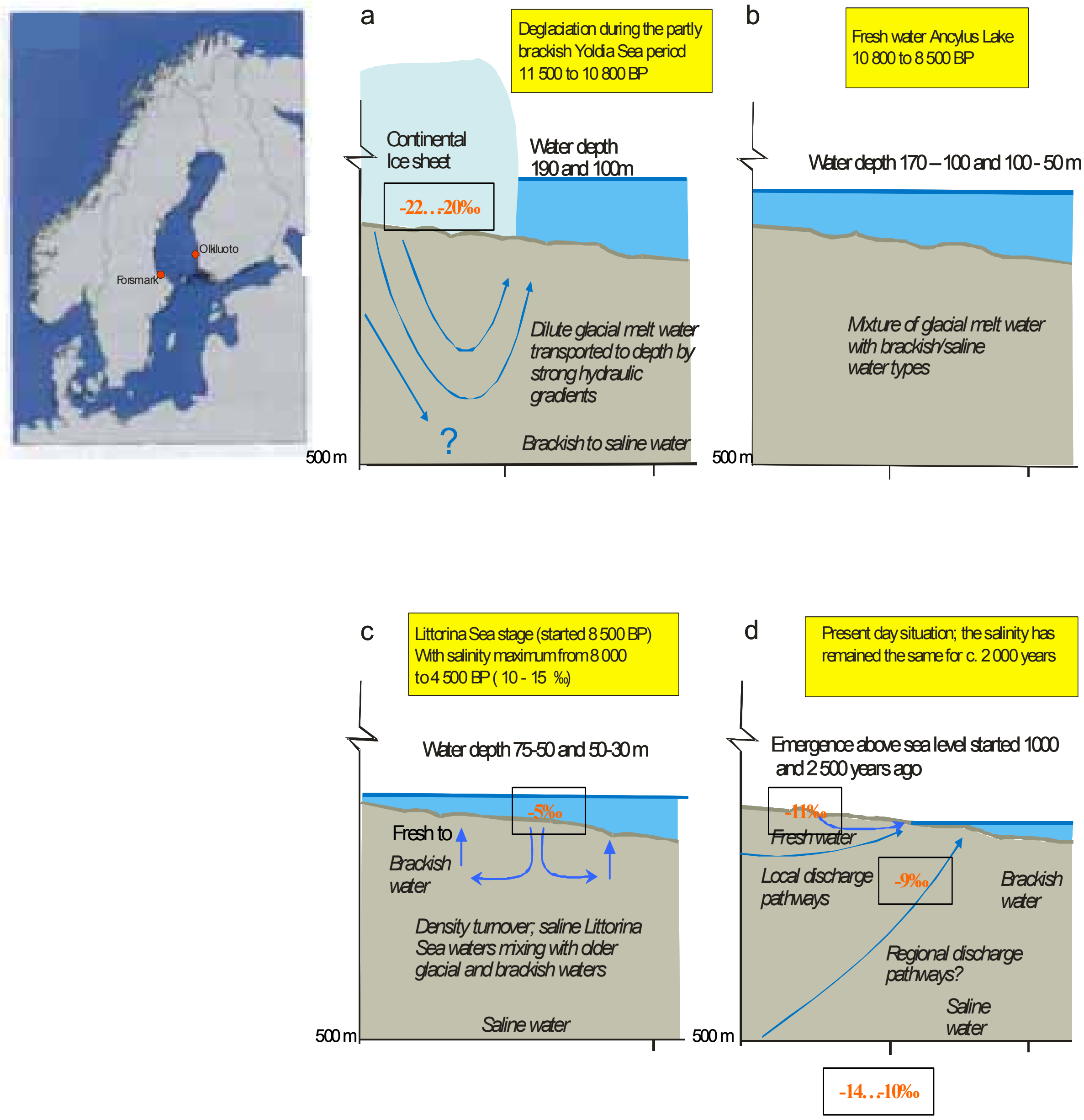
One of the main objectives of the Site Descriptive Models used by SKB (The Swedish Nuclear Fuel and Waste Management Company) in Sweden and POSIVA in Finland is to describe the chemistry and distribution of the groundwater in the bedrock and overburden and the processes involved in its origin and evolution. Through various cooperation projects the two companies have created models and understanding of the geohistory and the effects on the current groundwater features, conditions and possible future evolution but also an understanding of the limits of such modelling approaches [1, 2, 3, 4, 5].

The SKB/POSIVA hydrogeochemistry programmes are intended to fulfill two basic requirements: 1) to provide representative and quality assured data for use as input parameter values in calculating long-term repository safety, and 2) to understand the past and present hydrogeochemical conditions, and how these conditions will change in the future. Parameter values for safety analysis include pH, Eh, S, SO_4, HCO_3, PO_4 and TDS, together with colloids, fulvic and humic acids, other organics, bacteria and dissolved gases. The geohistorical evaluation and modelling requires an extensive geochemical data set including isotopic information. The groundwater values and their expected changes will be used to characterise the groundwater environment at, above and below repository depths. When the hydrogeochemical environment has been fully characterised, this knowledge, together with an understanding of the past and present groundwater evolution, will provide the basis for predicting future changes. The site investigations will therefore provide important source material for safety analyses and the environmental impact assessment of the studied areas.

The original understanding of groundwater evolution in fractured rock was based on models describing water rock interaction processes which did not take comprehensively into account geohistorical transport of different water types such as intrusion of ancient sea water. Consequently, the concept of necessary time scales and conditions for the reactions to produce the obtained groundwaters were questionable. In addition such descriptions could not be compared with hydrogeological modelling. During the site investigations in Sweden and Finland it was found that the hydrogeochemical evolution strongly results from flow, transport and water rock interactions driven by the past and present climate. As this is a continuous process, the type of infiltrating water as well as the existing groundwater will constantly change and will result in complex groundwater mixtures.

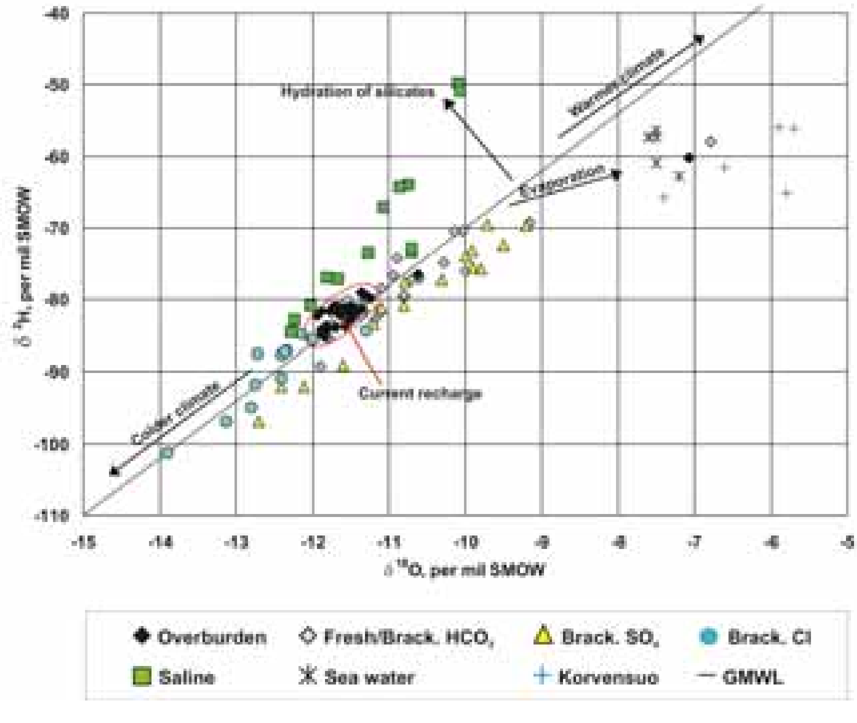
The understanding of the geohistory for the Fennoscandian sites is that during melting and retreat of the last ice sheet the following sequence of events is thought to have influenced the Swedish and Finnish sites such as Forsmark and Olkiluoto (Figure 1).

Figure 1. **Conceptual postglacial scenario model for the Swedish (Forsmark) and Finnish (Olkiluoto) sites (for orientation see the map). The figures a-d show possible flow lines, density driven turnover events and non-saline, brackish and saline water interfaces with indicative ^{18}O values (‰) of infiltrating water and current groundwater. The water depth and the time for the land emerging above sea level are indicated for Forsmark and Olkiluoto, respectively. Possible relation to different known postglacial stages such as land uplift which may have affected the hydrochemical evolution of the site is shown: a) deglaciation of the continental ice, b) Ancylus Lake stage, c) Littorina Sea stage, and d) present day Baltic Sea stage. From this conceptual model it is expected that glacial meltwater and deep and marine water of various salinities have affected the present groundwater.**



Many of the natural events described above may be repeated during the lifespan of a repository (thousands to hundreds of thousands of years). As a result of the described sequence of events, brine, glacial, marine and meteoric waters are expected to be mixed in a complex manner at various levels in the bedrock, depending on the hydraulic character of the fracture zones, groundwater density variations and borehole activities prior to groundwater sampling. This is also what can be seen in the chemical measurements of major components and isotopes which can be related to different climate driven events. As an example from Olkiluoto, Figure 2 shows the position of stable isotope compositions relative to the global meteoric waterline (GMWL) which can be used to indicate various chemical and physical conditions and processes associated e.g. with the geohistory. The isotopic composition of groundwater is in most cases controlled by meteorological processes and the shift along the GMWL reflects climatic changes in precipitation. Cold climate precipitation shows lighter isotopic compositions (more negative values), whereas warmer climate shows heavier composition. A shift to the right or below the GMWL typically indicates evaporation in surficial waters, which are enriched due to fractionation in heavier isotopes, particularly ^{18}O, relative to formed vapour. Therefore, for example the seawater composition is below the GMWL. The shift above the GMWL is unusual and observed mainly in shield brines. Such strong fractionation in oxygen and hydrogen isotopes may be due to effective primary silicate hydration under low water-rock ratio conditions.

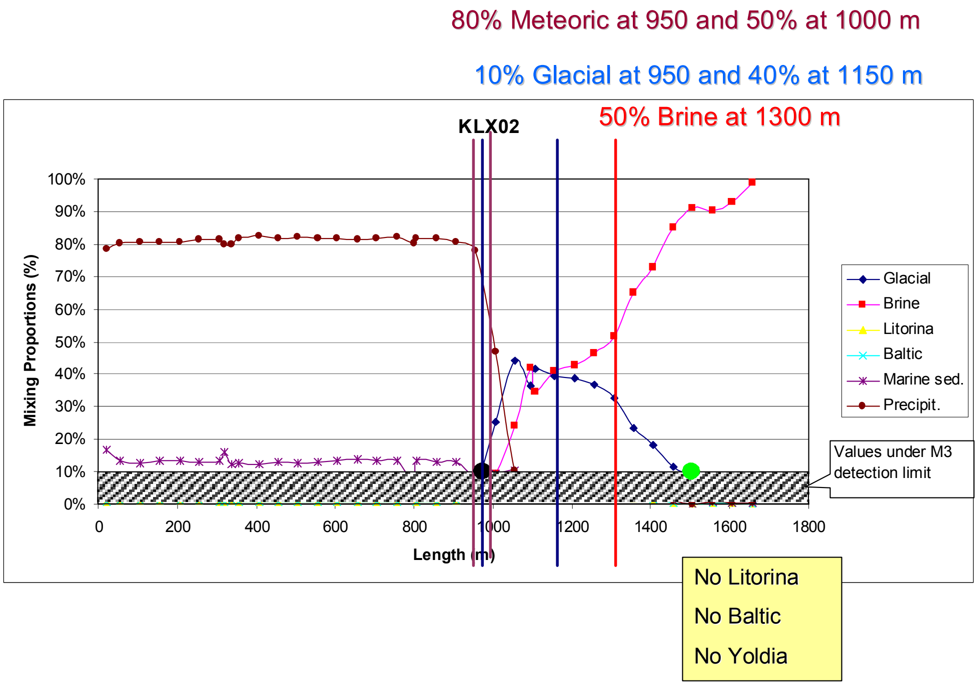
Figure 2. **Relationship between δ18O and δ2H in Olkiluoto groundwater samples. Arrows depict compositional changes caused by climate changes or water rock interaction. The Global meteoric water line (GMWL) is indicated.**



The solute and isotopic content of groundwater samples can be interpreted as either the result of geochemical reactions between the groundwater and the minerals it contacts, or as the mixing of groundwater types of different origins or end-members (and hence different chemical signatures). The SKB/POSIVA approach combines both processes. The information is decoded by using a multivariate statistical approach (M3) or by using the inverse modelling approach (PHREEQC) in combination with expert judgement. The mixing models are used to analyse variations in groundwater compositions so that the end-member mixing components, their proportions, and chemical reactions are revealed. The results of such interpretations can be combined or compared with independent hydrogeological descriptions of a site or used in calibrating hydrogeological simulations for achieving a consistent interdisciplinary model of a site. Integration provides an opportunity to improve our understanding of the hydrogeological performance of the repository site and to increase confidence regarding future predictions of its hydrogeological and hydrogeochemical evolution which is essential to the development of the safety case.

The present SKB and POSIVA modelling has further developed the comparison and integration between hydrochemistry and hydrogeology. Some hydrogeological models can be used to provide predictions, as a function of time, of the groundwater components and isotopes such as TDS, Cl, ^{18}O and ^{2}H in the immobile rock matrix water and in the mobile water flowing in fractures. Furthermore, the groundwater flow model can, independently from chemistry, predict the salinity at any point of the modelled rock volume, and the predictions can be checked by direct hydrogeochemical measurements or calculations. The mixing proportions from the hydrogeological model can, for example, be directly compared with the mixing calculations from the hydrogeochemical modelling (Figure 3).

Figure 3. **Example of comparison between hydrogeological and hydrogeochemical modelling along the depth (length) of the KLX02 borehole. The mixing proportions from the hydrogeological model (vertical lines) is compared with the M3 mixing calculations (curves) for borehole KLX02. The uncertainty of the M3 mixing proportions are in the order of ±10% from the reported value.**



At every phase of the hydrogeochemical investigation programme – drilling, sampling, analysis, evaluation, modelling – uncertainties are introduced which have to be accounted for, addressed fully and clearly documented to provide confidence in the end result, whether it will be the site descriptive model or repository safety analysis and design. The uncertainties can be conceptual uncertainties, data uncertainty, spatial variability of data, chosen scale, degree of confidence in the selected model, and error, precision, accuracy and bias in the predictions.

The following data uncertainties have been estimated, calculated or modelled for the Swedish groundwater data:

- temporal disturbances from drilling; may be ± 10-70%;
- effects from drilling during sampling; is <5%;
- sampling; may be ± 10%;
- influence associated with the uplifting of water; may be ± 10%;
- sample handling and preparation; may be ± 5%;
- analytical error associated with laboratory measurements; is ± 5%;
- mean groundwater variability during groundwater sampling (first/last sample); is about 25%.
- The M3 model uncertainty; is ±0.1units within 90% confidence interval

Conceptual errors can occur in, for example, the palaeohydrogeological conceptual model. The influence and occurrences of old water end members in the bedrock can only be indicated by using certain element or isotopic signatures. The uncertainty is therefore generally increasing with the age of the end member. The relevance of an end member participating in the groundwater formation can be tested by introducing alternative end member compositions or by using hydrodynamic modelling to test if old water types can reside in the bedrock during prevailing hydrogeological conditions. It is not always trivial to match the hydrogeological model to the chemical data, and vice versa. The chemical data could be rather insensitive to key aspects of the hydrogeological model (i.e. the flow characteristics in the repository volume), but very sensitive to other aspects – like the details of the near-surface hydrogeology or the initial conditions at the time of the past glaciation. Further enhancement of the interaction would be warranted, but it is also important to understand the practical limitations in achieving full integration.

The geohistory approach used by SKB and POSIVA can be used for explaining the measured major components and isotopes. The origin and the residence time of the groundwater can be indicated. The approach facilitates integration between hydrochemistry and hydrogeology. A well described site and the coupling with hydrogeology provides tools for predicting future groundwater changes affected by the climate. This fascinating exercise of predicting future groundwater conditions has just been initiated by SKB and POSIVA.

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TRANSFERABILITY OF FEATURES AND PROCESSES FROM UNDERGROUND ROCK LABORATORIES AND NATURAL ANALOGUES – USE FOR SUPPORTING SAFETY CASES IN ARGILLACEOUS FORMATIONS

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Abstract

It is current practice to transfer external information (e.g. from other sites, from underground rock laboratories or from natural analogues) to national safety cases. Transferable information most commonly includes parameters, investigation techniques, process understanding, conceptual models and high-level conclusions on system behaviour. Prior to transfer, the basis of transferability needs to be established. For argillaceous formations, the microstructure of the rocks, essentially determined by properties of clay minerals, provides such a basis in many cases. Examples are shown from the Swiss and French programmes how transfer of information was handled and justified.

1. Introduction

In several national programmes for the disposal of radioactive waste, argillaceous formations are considered as potential host rocks. The stages of development of the various programmes are quite different. Some programmes are at the stage of desk studies, others at the stage of generic investigations from the surface or from underground rock laboratories, and some have identified potential sites and initiated their characterisation. Given the differences in the degrees of development and sophistication, in technical focus and in project-relevant time scales, exchange of information and technical collaboration among the implementing organisations is very active. Aspects of common interest are investigated in national or international facilities such as the underground laboratories at Mont Terri (Switzerland), Mol (Belgium) and Bure (France). The NEA Working Group on Measurement and Physical Understanding of Groundwater Flow through Argillaceous Media (Clay Club) is another institution targeted at international collaboration. The Clay Club identified specific fields of interest and launched technical initiatives, such as:

- Water, gas and solute transport through argillaceous media (Horseman *et al.* 1996).
- Catalogue of Characteristics of argillaceous rocks (Boisson, 2005).
- Methods of sampling and interpretation of pore waters in argillaceous formations (Sacchi *et al.* 2000, 2001).
- Self sealing in argillaceous rocks (Horseman *et al. in preparation*).
- Features, Events and Processes Evaluation Catalogue for Argillaceous Media (FEPCAT, Mazurek *et al.* 2003).

- Natural tracer profiles across argillaceous formations – review and synthesis (CLAYTRAC, OECD/NEA, 2004).

While such co-ordinated actions increase the general process understanding and knowledge of the properties of argillaceous systems, the transfer of such information to specific sites is not trivial and needs to be done with care. This paper investigates two well characterised formations, namely the Callovo-Oxfordian at Bure (France) and the Opalinus Clay in northern Switzerland, and identifies properties and processes that may (or may not) be transferred from one formation to the other. In addition, transferability from natural analogues is addressed. A description of the methodology and the logic reasoning related to transferability is another important objective.

2. Basic site descriptions

2.1 Callovo-Oxfordian at Bure, France

In the eastern part of the Paris Basin, Andra is investigating a site near Bure (also called "Site Meuse-Haute Marne"), mainly targeting at a flat-lying, *ca.* 130 m thick argillaceous formation of Callovo-Oxfordian age at 420-550 m below surface. The area of investigation is characterised by very low seismotectonic activity. The formation and its embedding units are lithologically homogeneous in the lateral dimensions on a scale of tens of kilometres around the site, which indicates deposition in a tectonically quiet environment. Given the limited burial (*ca.* 850 m below surface) that occurred in the Cretaceous, diagenetic effects are weak and essentially limited to compaction and the formation of carbonate cement. Clay-mineral reactions, such as the partial illitisation of smectite, have not been identified. Brittle deformation is weak and mostly focused in known major faults that occur several kilometres away from the investigation site. The Callovo-Oxfordian is embedded by the Dogger and Oxfordian limestones, which contain horizons with aquifer properties.

Since 1991, the region has been extensively studied from the surface by 2-D seismic campaigns, a series of deep boreholes (with a total of 4 300 m of cores in the Callovo-Oxfordian) and a 3-D seismic campaign covering 4 km². Since August 2000, the construction of an underground research laboratory has led to the collection of *in situ* information during the shaft-sinking activities, completed by preliminary results of the excavation of galleries at 445 m below surface (upper part of the formation) and 490 m below surface (middle part of the formation). These investigations provided the basis for an extensive report (*Référentiel géologique*; Andra, 2005a), which is a part of the feasibility study for a geological repository at the investigated site. This feasibility study, called "Dossier 2005" (Andra, 2005b), is currently under evaluation.

2.2 Opalinus Clay at Mont Terri, Switzerland

The Mont Terri underground research laboratory is located in north-western Switzerland (Canton Jura) and consists of a dedicated tunnel section that branches off an existing motorway tunnel across the Mont Terri anticline in the Folded Jura Mountains. It is located in Opalinus Clay, a middle Jurassic marine shale formation, *ca.* 270 m below surface. At Mont Terri, Opalinus Clay occurs within an anticlinal fold and therefore is affected by brittle deformation. Research managed by the International Mont Terri Consortium was started in 1996 and is documented in Thury & Bossart (1999) and follow-up synthesis reports on geochemistry (Pearson *et al.* 2003), hydrogeology (Marschall *et al.* 2004) and excavation-disturbed zone/rock mechanics (Martin & Lanyon, 2002). In future, the main focus will be on long-term and demonstration experiments. Mont Terri is a generic underground facility and will not be considered as a disposal site.

2.3 Opalinus Clay in the Zürcher Weinland, Switzerland

In 1994, Opalinus Clay was identified as the priority sedimentary host rock option for the disposal of spent fuel and vitrified high-level waste in Switzerland, and the Zürcher Weinland (north-east Switzerland) as the first-priority area for site-related investigations. Detailed characterisation of the host rock and the potential siting area followed after 1994. The key elements of this research programme were a 3-D seismic campaign in the Zürcher Weinland covering an area of around 50 km^2, an exploratory borehole at Benken, experiments as part of the international research programme in the Mont Terri underground research laboratory, comparative regional studies on Opalinus Clay including deep boreholes in the near and far vicinity of the siting area, and comparisons with clay formations that are under investigation in other countries in connection with geological disposal. A synthesis report has been recently published (Nagra 2002a).

In the Benken borehole, Opalinus Clay is flat lying, essentially undeformed and occurs at a depth of 550-650 m below surface. It is not directly bounded by aquifers but embedded by lithologically more heterogeneous (even though often argillaceous) units. Natural tracer profiles of Cl and of water isotopes indicate that diffusion is the dominant transport mechanism between the late Jurassic and late Triassic aquifers, i.e. over a vertical distance of *ca.* 300 m (Gimmi & Waber, 2004).

3. Basic properties of the considered formations: Analogies and differences

The most relevant parameters of the formations under discussion are summarised in Table 1. The parameters of Opalinus Clay and the Callovo-Oxfordian show major similarities. It is remarkable that the porosities of these formations are similar in spite of the more limited maximum burial depth reached by the Callovo-Oxfordian. The reason probably lies in the diagenetic evolution, which involves a more pronounced cementation of the pore space (and hereby a reduction of porosity) in the Callovo-Oxfordian when compared to Opalinus Clay. This difference in burial and diagenetic evolution also explains the different anisotropy factors of diffusion coefficients and hydraulic conductivity (*ca.* 5 [De] and 1 - 10 [K] in Opalinus Clay and typically <2 for both De and K in the Callovo-Oxfordian), as well as some differences in the geomechanical properties. Both formations are slightly to moderately over-consolidated.

4. The basis of transferability

There are various levels on which information can be transferred to a specific safety case from other disposal programmes, underground rock laboratories and natural analogues:

- Individual parameters.
- Investigation techniques and data evaluation methods.
- Process understanding.
- Conceptual models.
- High-level conclusions (e.g. engineering feasibility, safety aspects).

Table 1. **Basic characteristics of the target formations**

Property / parameter	Callovo-Oxfordian at Bure	Opalinus Clay at Benken[(1)]	Opalinus Clay at Mont Terri
Depositional environment	shallow marine	shallow marine	shallow marine
Age	middle Callovian - lower Oxfordian, 158 - 152 Ma	Aalenian, 180 Ma	Aalenian, 180 Ma
Max. temperature reached during diagenesis [°C]	33 - 38	85	85
Present burial depth (centre [m])	488	596	275
Maximum burial depth (centre [m])	850	1650	1350
Over-consolidation ratio [-]	1.5 - 2	1.5 - 2.5	2.5 - 3.5
Thickness [m]	138	113	160
Clay minerals [weight-%]	25 - 55	54	66
Clay-mineral species (in the order of decreasing abundance)	Illite/smectite mixed-layers, illite, (chlorite, kaolinite)	Illite, kaolinite, ill/smec mixed-layers, chlorite	Illite, kaolinite, ill/smec mixed-layers, chlorite
Quartz [weight-%]	20 - 30	20	14
Feldspars [weight-%]	1	3	2
Calcite [weight-%]	20 - 38	16	13
Dolomite / ankerite [weight-%]	4	1	b.d.
Siderite [weight-%]	<1	4	3
Pyrite [weight-%]	1 - 2	1.1	1.1
Organic carbon [weight-%]	0 - 1	0.6	0.8
CEC [meq/100 g rock]	11 - 22	10.6	11.1
Pore-water type	Na–Cl-SO_4	Na-Cl-SO_4	Na-Cl-SO_4
Mineralisation [mg/L]	6530	12898	18296
Eh [mV]	< -150	-170	-227
Bulk wet density [Mg/m^3]	2.3	2.52	2.45
Water content [weight-% rel. to dry weight]	8.6	4.0	7.03
Physical porosity [-]	0.18	0.12	0.16
Geochemical porosity [-]	0.09	0.06	0.09
Total specific surface [m^2/g][(2)]	56 - 78 (BET H_2O)	90 (EGME)	130 (EGME)
External specific surface [m^2/g]	43 (BET N)	28 (BET N)	31 (BET N)
Eff. diffusion coeff. De (HTO) ⊥ to bedding [m^2/s], anisotropy factor[(3)]	2.6E-11 <2	6.1E-12, 5.0	1.5E-11, 4.7
Eff. diffus. coeff. De (Cl, Br, I) ⊥ to bedding [m^2/s], anisotropy factor[(3)]	1E-12 - 1E-11 anisotropy not measured (expected small)	6.5E-13, 5.0	4.1E-12, 6.1
Hydraulic conductivity K normal to bedding [m/s], anisotropy factor[(3)] [(4)]	5E-14 - 5E-13 small anisotropy (inside the range of variation)	2.4E-14, 5.0	4.0E-14, 5.0
Seismic velocity Vp [m/s]	3000 - 3200 (⊥), 3200 - 3400 (//)	3030 (⊥), 4030 (//)	2620 (⊥), 3030 (//)
Uniaxial compressive strength ⊥ to bedding [MPa]	20 - 35	30	26
Young's modulus (static, normal to bedding) [MPa], anisotropy factor[(3)]	4500 - 7000, 1.3	5500, 2.1	9500, 1.6
Cohesion normal to bedding [MPa]	6.4	1.9	2.2
Angle of internal friction normal to bedding, [°]	29	24	23
Swelling pressure [MPa]	1.0 - 3.0 (anisotropy not measured)	1.1 (⊥), 0.15 (//)	1.2 (⊥), 0.5 (//)

(1) Including Murchisonae Beds in Opalinus Clay facies

(2) Specific areas derived from BET (H_2O) are typically smaller than those measured by EGME on the same samples. Therefore, the values are only comparable when based on the same methodology

(3) Anisotropy factor = value parallel / value normal to bedding

(4) The numbers given for Opalinus Clay are the reference values, but the range of uncertainty is substantial

Data sources: Andra (2005a), Boisson (2005), Nagra (2002a).

In argillaceous systems, the microscopic structure governs many macroscopic properties, including, among others, transport and geomechanical properties. Microstructure is essentially determined by clay-mineral platelets with grain sizes of a few µm or less, arranged in a network of plate-to-plate and edge-to-plate contacts. This network results in high surface areas and in an equally complex geometry of the interstitial space, i.e. the water-filled porosity, which is characterised by apertures in the range of nm. This type of microstructure is common to all argillaceous systems and is the fundamental basis of transferability among different sites and formations.

However, some differences occur among argillaceous formations and are mainly due to variations of the

- degree of compaction (and therefore porosity);
- degree of diagenetic cementation;
- contents of coarser-grained clastic material, such as quartz and carbonate minerals;
- *in situ* stress regime, in specific the magnitude of shear stress.

Thus, good knowledge of mineralogy, of diagenetic evolution and of tectonic, burial and thermal history is another foundation of transferability. Mineralogy and porosity are the most important characteristics to be considered for the transfer of data and processes among different argillaceous systems.

4.1 Why do we want to transfer features, processes and know-how, and at which stage?

National programmes are at quite different stages of development (desktop study, borehole data, underground facilities) and also pursue country-specific strategies of developing a safety case. There are the following major motivations for the transfer of information among formations/sites:

1. Information from other sites is taken to fill current gaps in a specific national programme, in order to obtain data for a preliminary safety case. For example, the basis for extrapolating laboratory measurements to *in situ* conditions can be justified if both laboratory and *in situ* data are available in other programmes. As an example, comprehensive data bases such as the Clay Club Catalogue of Characteristics (Boisson, 2005) or the catalogue of features, events and processes for argillaceous systems (FEPCAT, Mazurek *et al.* 2003) can be used to transfer findings from other programmes.
2. Information from other sites is taken to highlight that the investigated formation and/or site does not represent an exceptional situation but has relevant features in line with other argillaceous formations. If independent programmes converge towards consistent data sets and conclusions, confidence is built in the national programme. Examples: Demonstration of diffusion as the dominant transport process, of the efficiency of fault self sealing, of the hydraulic irrelevance of faults, of reducing geochemical environments, *etc.*
3. On the other hand, the identification of evident differences can be used to guide future research. Example: Possible presence of highly saline pore waters in the Ordovician shales underlying southern Ontario, consequences for the accessibility of the pore space to solutes, on solute-clay interactions and on geochemical modelling.
4. Dedicated investigation techniques are often developed and evaluated in underground rock laboratories and then used for site characterisation elsewhere. Practical examples include, among others, the instrumentation for in-situ diffusion experiments and the development of geotechnical equipment.

5. Conceptual models on different levels (individual features and processes, their coupling and safety relevance) can be transferred from other, similar sites or underground rock laboratories. Examples include the identification of relevant transport processes in the geosphere and the role of natural and induced fractures on flow and transport.

In practice, point 1 above is more relevant in the early stages of developing a safety case, while point 2 becomes more important in mature safety cases. The more mature a safety case, the less information is borrowed from elsewhere, and the more are external data and conclusions used as additional, independent lines of evidence. Points 3 and 4 are important throughout the whole process of making a safety case.

Natural analogues are used as independent lines of evidence for safety cases in all stages of development. The strength of natural analogues lies in the fact that they record processes that occurred over large scales in space and time, often comparable with those needed for PA, and thus are helpful for the upscaling of experimental work conducted in the laboratory or in underground research facilities (see reviews by Alexander & McKinley 1992, McKinley & Alexander 1992, Miller *et al.* 2000). However, the transferability of information from natural analogues to specific repository sites is limited by a number of weaknesses, such as, *inter alia*, the difficulty to constrain the age, duration and interplay of relevant processes, significant differences in the geological settings, the boundary conditions and their evolution with time. Due to these limitations, a substantial part of the transferable information is qualitative in nature, even though not exclusively.

4.2 What can be transferred, what cannot, and how?

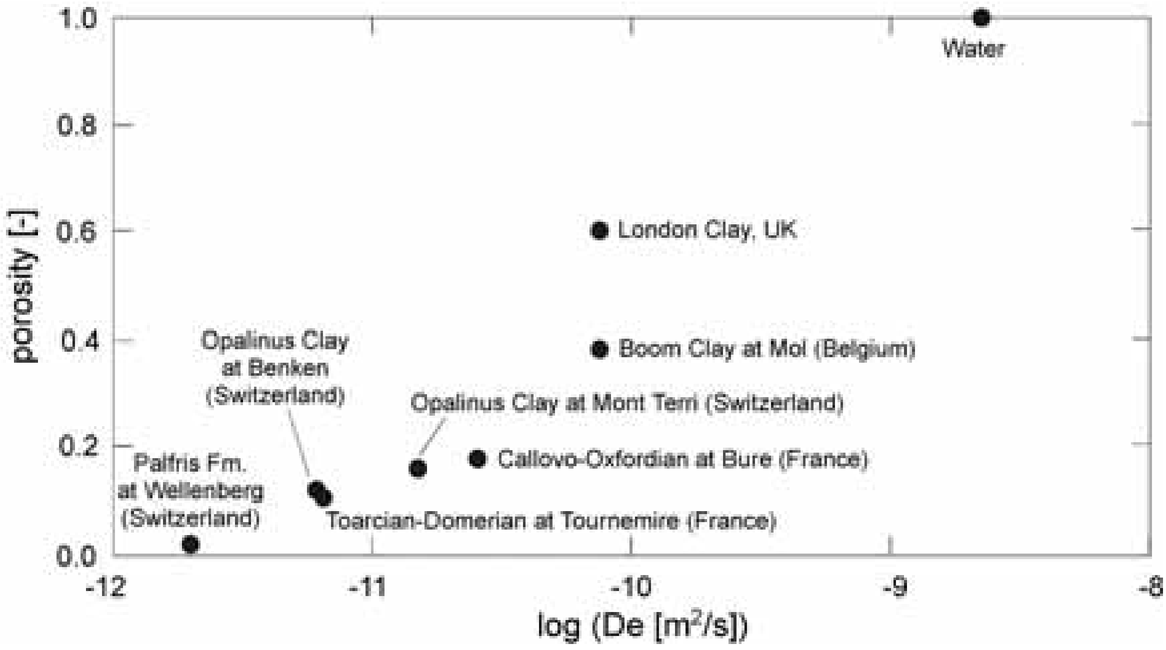
As discussed above, mineralogy and porosity are among the most important macroscopic parameters of argillaceous systems. Many parameters and processes are functions mainly of mineralogy and porosity, and the understanding of this dependence is an important pre-requisite for transferability. In principle, the following types of features and processes can be distinguished:

- Features and processes that do not strongly depend on known or expected differences between different argillaceous formations; e.g. thermodynamic or kinetic data used to quantify water/rock interactions.
- Features and processes that essentially depend on mineralogy and porosity only but only insignificantly on the state of the system (*in situ* stress, hydraulic head, temperature, salinity); e.g. permeability, thermal conductivity and some geomechanical properties. The dependence on mineralogy and porosity requires detailed characterisation, and this is often linked to a thorough knowledge of the geological evolution of the sites involved.
- Features and processes that essentially depend on mineralogy and porosity but also on other properties and on the state of the system; e.g. diffusion and sorption properties (also depending on pore-water composition and temperature), geometry and extent of the excavation disturbed zone (EDZ) around underground structures. In cases where the understanding of complex system behaviour has to be transferred into another environment (e.g. the geometry and the properties of the EDZ around tunnels in the target area, where no direct observations are currently available), transferability is more complex and appropriate conceptual models, computational tools and parameter sets have to be used in order to assess the combined effect of rock properties and site-specific conditions.
- Features and processes that depend substantially on the state of the system; e.g. hydraulic head and gradient, salinity of pore and ground water. For such data, site-specific information is essential and transferability is generally not possible. In safety assessment, long-term evolution scenarios have to be considered for such parameters.

Example 1: Diffusion coefficients

As shown in Figure 1, for argillaceous rocks, there is an empirically well defined relationship between the logarithm of the effective diffusion coefficient and porosity. A similar relationship can also be seen for the logarithm of the pore diffusion coefficient and porosity (essentially reflecting the fact that Archie's law is largely applicable). It follows – as an empiric conclusion – that compaction of an argillaceous formation reduces both porosity and tortuosity in a regular way. If porosity is known, diffusion coefficients can be estimated on the basis of this correlation.

Figure 1. **Effective diffusion coefficient of tritium (normal to bedding) in various argillaceous formations.**

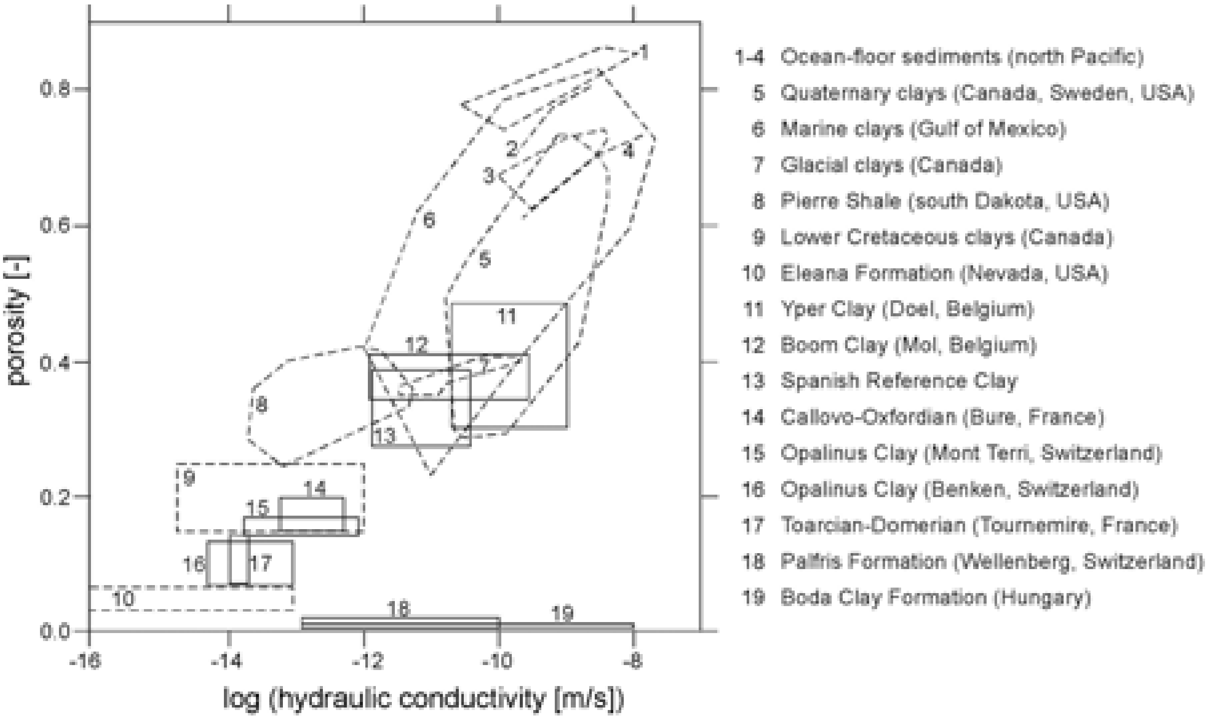


Data from Andra (2005c), Atkins (1990), Boisson (2005), Bourke *et al.* (1993), Lineham & Stone (1991) and Nagra (2002a).

Example 2: Hydraulic conductivity

Figure 2 shows that there is a positive correlation between porosity and the logarithm of hydraulic conductivity for porosities larger than *ca.* 0.05 – 0.1. However, for highly compacted (and, at the depth of observation, also strongly over-consolidated) formations with smaller porosities, the trend is broken, and effective hydraulic conductivity may increase sharply. This is probably due to the fact that matrix permeability becomes insignificant when compared to fracture permeability. Severe over-consolidation and fracturing typically occur in highly compacted systems that have lost their plasticity and part of their self-sealing capacity due to the more limited occurrence of swelling clay minerals. Therefore, the transferability of hydraulic conductivity and some other parameters is limited, at least in highly compacted systems. There is no single porosity value below which fracture permeability becomes dominant, as other features, such as over-consolidation ratio, stress regime, cementation, self-sealing capacity *etc.* also play a role.

Figure 2. **Hydraulic conductivity in various argillaceous systems.**



Data sources - Formations 1-10; Neuzil (1994), shown in dashed lines; formations 11-13, 17-19: Boisson (2005); 14: Andra (2005c); 15-16: Nagra (2002a). Note that data without a documented experimental protocol in Neuzil's (1994) compilation were not considered.

5. Practical experience with transferability

5.1 Andra's Dossier 2005 for the Site Meuse-Haute Marne (Bure)

Andra gained substantial experience from experimental work carried out in the underground rock laboratories at Mol (over the last 20 years) and Mont Terri (since 1996). The main points include:

- the development of experimental tools and methods;
- questions related to scale issues;
- the development of conceptual models;
- testing the comprehensiveness of the site characterisation and safety approach.

Development of experimental tools and methods

The availability of tested experimental tools and protocols before and during the development of the experimental programme at the Meuse-Haute Marne site resulted in a substantial gain of time. Examples, all documented in Andra (2005 a,b), include:

- Design and dimensioning of the DIR experiment (*in situ* diffusion test) in the Bure underground laboratory were based on an analogous experiment (DI) at Mont Terri (Palut *et al.* 2003, Tevissen *et al.* 2004).

- Geotechnical instruments, such as extensometers and inclinometers, were originally developed at Mol (CLIPEX experiment, Bernier *et al.* 2003) and are now used for the REP experiment (shaft sinking response) at Bure.
- The feasibility and hydraulic performance of a concept considering the cutting of radial trenches into the tunnel walls, thereby removing the EDZ, and subsequently backfilling them by bentonite bricks, was tested in the EZ-A ("EDZ cut-off") experiment at Mont Terri in 2003 and 2004 (Armand, 2004). Focus was placed on 1) the study of possible mechanical damage due to trench excavation, 2) feasibility of bentonite emplacement, and 3) testing the hydraulic performance of the seals by cross-hole packer tests. This successful experiment was used to design and dimension the KEY experiment in the Bure underground laboratory, which will run over extended periods of time in order to achieve full saturation of the bentonite. A custom saw has been built to cut trenches up to 2.7 m deep into the tunnel walls.

Scale issues

Information from Mont Terri has also been used for scale issues. At Mont Terri, diffusion coefficients for various species (HTO, ^{36}Cl, I, ^{22}Na) were measured both in the laboratory (through-diffusion cells; Van Loon *et al.* 2002, Tevissen *et al.* 2004) and *in situ* (DI and DI-A experiments; Palut *et al.* 2003, Tevissen *et al.* 2004, Van Loon *et al.* 2004, Wersin *et al.* 2004). The latter characterise scales in time and space at least 1 order of magnitude greater than the laboratory data. The resulting coefficients were very similar for a given solute, which was taken as evidence that the scale dependence is small. This conclusion was used to justify the use of laboratory-derived diffusion coefficients for the Callovo-Oxfordian at Bure for larger scales. Use of this conclusion was made both for the design of the currently ongoing *in situ* test at Bure and for preliminary modelling of solute migration on the site scale (Andra 2005a).

Conceptual models – examples pertinent to the role of transport along brittle discontinuities

The general contention that fractures in argillaceous media are infrequent and/or hydraulically insignificant is one of the main arguments for considering these rocks for waste isolation. Andra used observations and conceptual models from Mont Terri to better justify this contention in the safety argumentation for the Bure site, regarding both artificial fractures in the EDZ as well as natural fractures.

A preliminary conceptual model for the geometry and hydraulic significance of the EDZ around the tunnels in the Bure underground laboratory was needed at a stage when no site-specific measurements were available. Given the different settings and degrees of compaction of Opalinus Clay at Mont Terri and the Callovo-Oxfordian at Bure, the *in situ* stress field and the degree of anisotropy of geomechanical properties are distincly different (Table 1), and some differences are also identified in strengths and moduli. Therefore, a direct transfer of observations and measurements pertinent to the EDZ at Mont Terri was not feasible, and the current conceptual model of the EDZ at Bure is based on data derived from geomechanical laboratory experiments and subsequent modelling. However, the same modelling approach was successfully used to predict the EDZ geometry at Mont Terri (using local parameters), and this adds confidence to the overall validity of the chosen approach (Andra 2005a). In the same way, the evaluation of the initial EDZ permeability was assessed taking into account the information from Mont Terri (Andra 2005c).

Another conceptual aspect is the time evolution of the EDZ, which has not yet been investigated at Bure. Given the fact that swelling pressures of Opalinus Clay and the Callovo-Oxfordian are comparable, the self-sealing behaviour can be assumed to be similar. Accordingly, the characterisation of fracture closure and related reduction of EDZ permeability with ongoing resaturation of the host rock and of the bentonite backfill at Bure was guided by the observations made at Mont Terri (Andra, 2005a,c).

A similar argument can be made regarding self sealing of natural fractures and faults. Various types of brittle discontinuities were identified at Mont Terri, while, to date, they have not been found at Bure (and, due to the different tectonic evolution, possibly will not be found even when tunnel observations will become available). At Mont Terri, observations and measurements indicate that natural brittle discontinuities of all types are hydraulically insignificant (unless part of the EDZ). This is true for small fractures as well as for major faults with extents of more than 100 m, indicating that self sealing is very efficient (Marschall *et al.* 2004; Andra 2005a). The absence of observed fractures at Bure, together with the efficient self sealing observed at Mont Terri, was the basis for disregarding fractures as potential flow conduits in solute transport calculations at Bure (Andra, 2005c).

Comprehensiveness of the safety approach

Andra's approach to safety analysis (Andra, 2005d) considers an inventory of the risks and uncertainties, called "Qualitative Safety Analysis" (AQS). In this analysis, available international FEPs (features, events and processes) data bases, such as the OECD/NEA data base (OECD/NEA, 2000), the results of the FEPCAT project (Mazurek *et al.* 2003) and the Swiss database for Opalinus Clay (Nagra, 2002b) were also considered. Establishing a link between each FEP and each part of the analysis was a procedure that implied a detailed test of the safety argumentation. This procedure was useful to verify and clarify the qualitative safety analysis and also provided supplementary information on several aspects (e.g. "external" events). The final comparison between the qualitative safety analysis and international data bases and ways of safety reasoning showed that the AQS is comprehensive and logically structured in an international context, and this factor adds credibility to the Dossier 2005 as a whole.

5.2 Gas transport mechanisms in Opalinus Clay: Lessons learnt at Mont Terri

Gas transfer from the emplacement tunnels through the host rock has been recognised as an important issue in Nagra's assessment of long-term safety of an SF/HLW/ILW repository in Opalinus Clay of northern Switzerland. High emphasis was therefore given to the elaboration of a well-founded, defensible data base on gas-related properties of the host rock. The investigations concentrated on the deep borehole at the candidate repository site in the Benken area, and on the Mont Terri rock laboratory (Nagra 2002a, Marschall *et al.* 2005). The approach consisted of the following steps:

- collect site-specific data bases on gas-related rock parameters;
- develop structural and process models of gas transport in Opalinus Clay and check their applicability to both sites;
- check consistency of parameters and concepts with information from elsewhere and derive generalised empirical relationships.

The opportunities for gas-related investigations at Benken were quite restricted due to the technical constraints associated with deep borehole investigations (poor borehole stability, limited accessibility of host rock, demanding core sampling procedures) and due to the tight time schedule of the geoscientific investigation programme. One single *in situ* gas injection test was performed, complemented by two long-term gas permeability tests on core specimens and a variety of microstructural analyses (e.g. nitrogen and water adsorption/desorption, mercury porosimetry). The corresponding programme at Mont Terri was more comprehensive both in extent of testing and experimental sophistication (including *in situ* experiments with extensive hydro-mechanical crosshole instrumentation and gas permeability tests on high quality rock specimens, recovered with advanced core sampling procedures, in order to minimise sample disturbance). The challenge was to combine the strengths of the two data sets by a traceable geoscientific methodology, which links both the conceptual understanding of gas transport mechanisms and the gas related parameters from Mont Terri to the geological conditions at Benken.

The development of process models was based on the fact that gas transport in low-permeability formations is largely controlled by the microstructure of the rock. The pore space of Opalinus Clay at both sites is formed essentially by a network of micro/meso- and macropores with effective pore throats in the order of 1-100 nm. Even though the tectonic regime at Mont Terri is distinct and includes fractures and faults, these do not contribute significantly to the bulk permeability of the rock due to efficient self sealing (Marschall *et al.* 2004). Further, minor differences between the two sites include the slightly lower clay-mineral content and higher degree of compaction at Benken when compared to Mont Terri (Table 1), which results in a somewhat different geomechanical behaviour.

The phenomenological description of gas transport processes in Opalinus Clay has been driven by the above mentioned microstructural conceptualisation of the rock (Figure 3a), suggesting the following basic transport mechanisms:

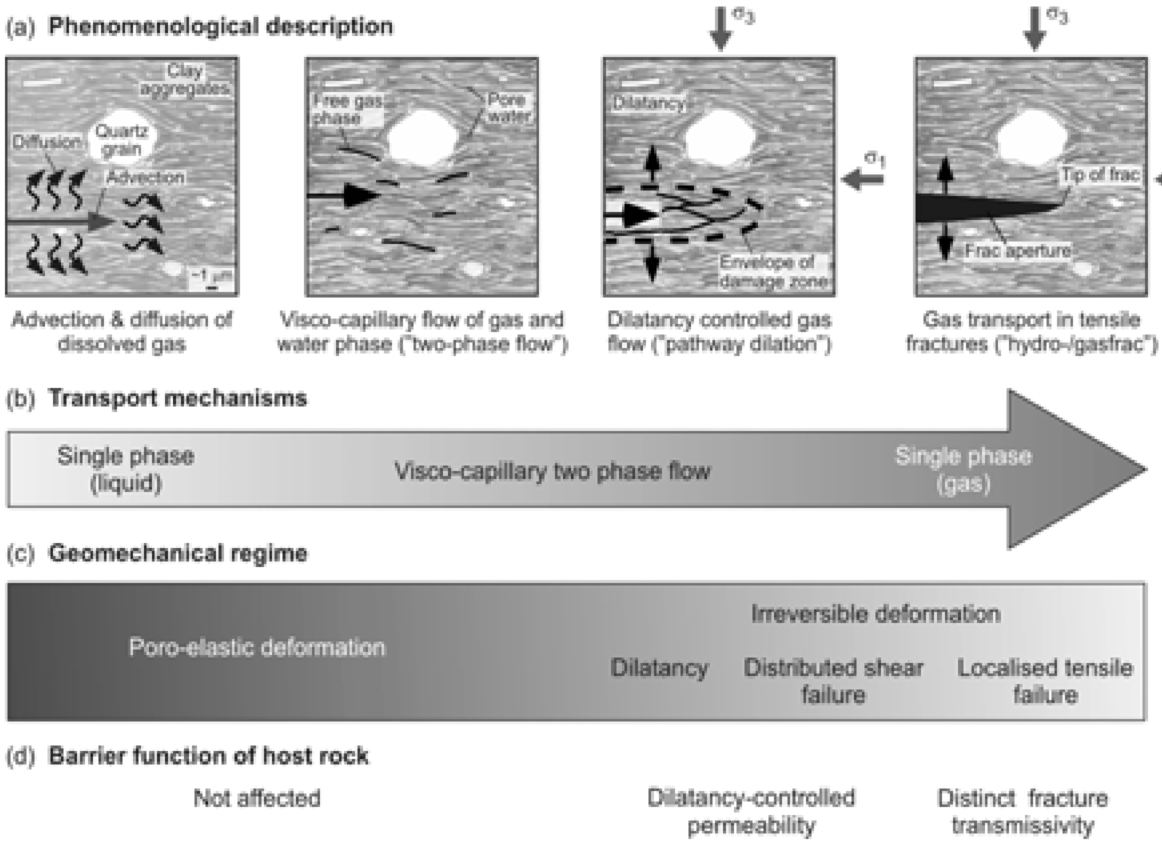
- advective-diffusive transport of gas dissolved in the pore water;
- visco-capillary two-phase flow;
- dilatancy controlled gas flow (“pathway dilation”);
- gas transport along macroscopic tensile fractures (hydro- and gas fracturing).

The complex hydro-mechanical processes of gas transfer through the rock can be decomposed into a problem of flow of immiscible fluids (Figure 3b) and a geomechanical problem (Figure 3c). Comprehensive theories are available in hydrogeology to describe flow of immiscible fluids (multiphase flow) in porous media. Similarly, a multitude of material laws have been developed in the field of geomechanics for modelling both ductile and brittle behaviour of geotechnical media. In Nagra’s gas-related studies, experimental evidence was needed to describe the postulated transport processes and geomechanical material laws. The corresponding data base was gained by a targeted hydrogeological and geomechanical investigation programme at Mont Terri (Marschall *et al.* 2005) and confirmed by checking the consistency of experimental results with the available data from Benken. The comparison of results comprised a broad spectrum of aspects such as clay contents, pore size distributions, capillary pressure curves, gas permeability measurements, stress-strain relationships and rock failure modes.

Gas permeabilities and gas entry pressures are somewhat different at Benken ($k = 1E\text{-}21 - 7E\text{-}21$ m^2, $p_{ae} = 4 - 10$ MPa) and Mont Terri ($k = 1.5\ E\text{-}20 - 6E\text{-}20\ m^2$, $p_{ae} = 0.2 - 1$ MPa). The differences can be satisfactorily explained as mainly due to slightly different degrees of compaction (and therefore porosity and pore-size distribution), of the *in situ* stress field and of clay-mineral content. The negative correlation between permeability and gas entry pressure as seen in Opalinus Clay at the two investigated sites is what would be expected on the basis of theoretical considerations. Qualitatively, the correlation corresponds to empiric trends derived from various studies in other formations (Davies 1991, Ingram *et al.* 1997), and this adds further confidence in the results.

Comparing the gas transport characteristics of Opalinus Clay with the expected production rates of repository gas, it is concluded that the dominant gas transport mechanism will be two-phase flow with a possible contribution of dilatancy controlled gas flow, whereas no gas fracs are expected to occur in the potential siting area.

Figure 3. **Classification and analysis of gas transport processes in Opalinus Clay after Marschall *et al.* (2005): (a) phenomenological description based on the microstructural model concept, (b) basic transport mechanisms, (c) geomechanical regime and (d) effect of gas transport on the barrier function of the host rock**



5.3 The Jordanian cementitious natural analogues

A full review of the transferability of natural analogues *per se* is outwith the remit of this paper. One example is chosen, namely the interaction of cement leachates (from a cementitious repository) with an argillaceous host rock.

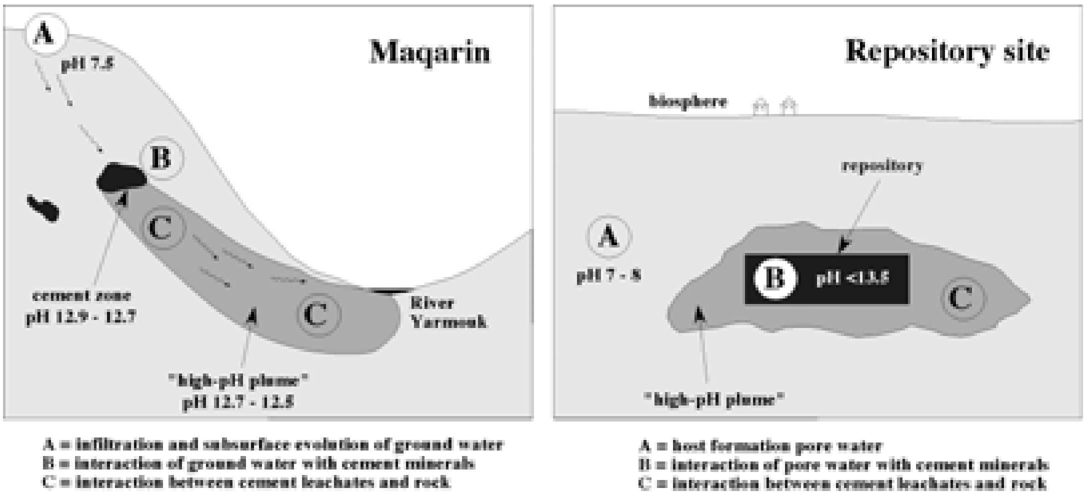
Basis of the analogy

The Jordanian cementitious natural analogue consists of three main sites: Maqarin in northern Jordan (on the border with Syria), Daba in central Jordan and Kushaym Matruk in south-central Jordan. At all sites studies, natural cement minerals were produced as a result of a high temperature-low pressure metamorphism (fueled by the *in situ* combustion of organic matter) of the marls and limestones of the area (Khoury *et al.* 1992). At Daba and Kushaym Matruk there are no current groundwater flows but, at Maqarin, hyperalkaline ground waters (pH 12.5 to 12.9) occur as products of leaching of the cement minerals. These waters are similar to early and evolved cement leachates in a repository system.

At Maqarin, the hyperalkaline waters infiltrate the adjacent clay-mineral bearing limestones along fractures and interact with the wallrocks along the flow path. This process is taken as an analogue to the possible high-pH plume that may develop downstream from a cementitious repository (see Figure 4). In particular, the situation is analogous to a repository located in fractured host rocks, or it can be conceived as an analogue of transport in the EDZ or in hypothetical fractures that may be considered in alternative PA scenarios of an otherwise unfractured host rock. Allied to the cement mineralogy is the fact that the formation also contains high concentrations of a suite of trace elements of interest to a repository safety assessment (including U, Se, Ni, Ra, Sn *etc.*), making the site a particularly apt analogue of a cementitious repository (Alexander *et al.* 1992). Detailed documentation on Maqarin can be found in Alexander (1992), Linklater (1998), Smellie (1998) and Pitty (*in prep.*).

The microstructure of the limestone at Maqarin, which is poor in clay minerals, is different from that in argillaceous media. While geochemical behaviour depends less on microstructure and so can be transferred, hydrogeological or geomechanical characteristics are not transferable.

Figure 4. **Basis of the analogy between the high-pH plume at Maqarin and a cementitious repository. Not to scale. Size and shape of the plume around a repository are site specific (fractured vs. diffusion-dominated system, EDZ structure, etc).**



Interaction between hyperalkaline water and wall rock at Maqarin

The predicted mineralogical evolution of the hyperalkaline plume in a host rock (both fractured and non-fractured; e.g. Savage 1998) is largely consistent with observations of secondary minerals at the Maqarin site, indicating that the mineralogical information is likely to be transferable. Consequently, model calculations considering reactive transport (coupled flow and chemical reaction between hyperalkaline water and rock, including reaction kinetics) were performed in order to estimate the possible effects of hyperalkaline plumes on other host rocks (e.g. Steefel & Lichtner 1994, 1998; Soler, 2003). Some of these calculations predicted massive dissolution of the rock matrix along fractures and, at the same time, the formation of a zone with zero porosity in the distal part of the alteration rims in the matrix due to the precipitation of calcite. Such a situation would be critical from a PA perspective because it increases fracture apertures (and thereby fluxes) and at the same time seals off the matrix (thus limiting the extent of the diffusion-accessible matrix). However, the model calculations have some weaknesses, such as the uncertainty related to thermodynamic and kinetic data and to the choice of underlying conceptual model (geometry, evolution of water at the inlet with time, porosity change over time). Evidence from Maqarin can reduce some of these uncertainties:

- Reactions between hyperalkaline waters and wall rocks occur extensively and within short time scales (years to hundreds of years). In this aspect, observations and model predictions agree.
- Most reactions have positive reaction volumes, and fractures are sealed by the precipitation of new solid phases, such as CSH gels or zeolites. Fracture sealing decreases hydraulic conductivity and so attenuates the alteration process. These observations disqualify model calculations predicting strong matrix dissolution and an enhancement of fracture apertures.
- Fracture infills at Maqarin often show recurrent events of fracture opening (due to tectonic or gravitational movement of the rock mass) and fracture sealing (up to a dozen stages of fracture infilling can be observed in a single fracture). This observation underpins the capacity of the system for self sealing.
- In agreement with model predictions, a zone of reduced porosity (0.05-0.1, compared to 0.4 in unaltered rock) occurs in the frontal parts of the alteration rim in the rock matrix. However, there is no evidence of complete sealing (zero porosity), and some traces of hyperalkaline water/rock interaction are also observed ahead of this zone.

On the other hand, there are also limitations to the transferability of the findings at Maqarin to argillaceous repository sites:

- Maqarin is a surface-near system with hydraulic conductivities and fluxes several orders of magnitudes higher when compared to deep argillaceous formations. This means that advection dominates over diffusion. The observed length of the plume (hundreds of metres) and penetration depth of alteration into the rock matrix (millimetres to centimetres) are not representative for most repository situations.
- Maqarin is a sub-oxic to oxic system, in contrast to most deep argillaceous systems that are strongly reducing. Secondary mineralogy at Maqarin includes several phases containing sulphate, such as ettringite and thaumasite, which are not expected in a repository situation due to the limited availability of sulphate (essentially derived from pyrite oxidation). Further, the observed concentration and (im)mobility of redox-sensitive solutes (including several radionuclides) may not be transferable to repository sites.
- Wall-rock mineralogy at Maqarin is dominated by calcite, with only small proportions of silicates (mainly clay minerals). This has to be borne in mind when transferring data and conclusions to the much more silicate-rich mineralogies of repository sites.

Further potential applications of the Maqarin natural analogue for repository sites include the study of trace-element geochemistry (Linklater *et al.* 1996), microbial activity under hyperalkaline conditions (West *et al.* 1995), of colloid formation and transport, and the geochemical behaviour of organic material.

Lessons learnt from Kushaym Matruk

For unfractured argillaceous media in which self sealing of the EDZ occurs rapidly (such as the Boom Clay; Barnichon & Volckaert 2003, Mertens *et al.* 2004), the transferability of findings at Maqarin is more limited, and the Kushaym Matruk site in south-central Jordan appears to be more appropriate. Here, the limestone in which interactions with hyperalkaline leachates occurred is less fractured and possibly represents a diffusive system, with slow movement of the leachates through the limestone matrix (Techer *et al.* 2004, Trotignon *et al.*, *in prep.*). The clay content is higher (3-16 wt%) than at Maqarin, which is another favourable feature. Rassineux (2001) identified a decrease of the crystallinity of clay minerals and of smectite content in illite/smectite mixed-layers, as well as the formation of zeolites. Although site interpretation is complicated by the existence of a thermal overprint (from the organic material combustion) and by fracturing that postdates the hyperalkaline interactions, the geochemical data are consistent with the Maqarin model and a recent laboratory study of cement leachate interaction with material from the Callovo-Oxfordian formation at Bure (Ramirez *et al.* 2005), suggesting the site may reward further study. Studies aimed at dating the hyperalkaline interactions are useful for long-term considerations (>100 ka; Andra 2005a).

6. Conclusions

6.1 General

Transfer of external data and concepts as input to national safety cases is an important element of confidence building. The basis of transferability as well as its limits need to be elaborated and justified in each specific case, and it may vary substantially among the different groups of host rocks (*e.g.* argillaceous and crystalline rocks, salt formations). Depending on the nature of the feature or process in question, this basis is established by the characterisation, understanding and comparison of:

- relevant formation properties (such as microstructure, mineralogy, porosity, redox conditions), and/or
- the states of the system (such as stress state and pore pressure)

in the concerned sites/formations. In many cases, it can be shown empirically that the feature or process to be transferred is essentially a function of a limited number of formation properties (for example, diffusion coefficients in argillaceous rocks depend mainly on porosity). In such cases, the basis of transferability is the characterisation of the empirical relationships. Further confidence in this methodology is gained by including data and insights from other sites and formations over and above those among which the transfer takes place.

Transfer occurs at different levels, depending on 1) the degree of development of the safety case and 2) the goodness of the analogy that can be made between the sites and formations concerned. In the early stages of a safety case development, information is transferred from other sites to fill current gaps in site characterisation and obtain a data set needed for a preliminary safety case. At this stage, the basis of transferability may not be well elaborated. In mature safety cases, the role of information transfer is less to supply missing data but to contribute to process understanding and confidence building, for example by means of establishing empirical relationships that include information from diverse sites and settings.

In summary, it is concluded that transfer of information, whether explicitly or implicitly, occurs at all stages in the development of a safety case and includes data from specific similar sites (repository sites, underground rock laboratories, natural analogues) but also the much larger (even though less similar) body of external information documented in the open literature.

6.2 Conclusions specific to argillaceous rocks

The main commonalty of argillaceous rocks (and therefore the most commonly applicable basis of transferability) is the presence of clay minerals with their distinct properties that determine a number of relevant features and processes, such as:

- Advection and diffusion of water and gas depend on the structure of the pore space (interconnected network on a nanometric scale), which in turn is determined by the spatial arrangement of clay platelets.
- Sorption is mainly determined by the high specific surfaces and reactivity of clay minerals.
- Self sealing of fractures depends on the swelling properties of clay minerals and on the strength of the rocks.
- Geomechanical properties, such as strengths and *moduli*, depend on the nature of the minerals as well as on the microstructure of the pore space and its water content.
- The degree of anisotropy of transport and geomechanical properties is linked to the bedding-parallel alignment of clay platelets.

Transferability is more restricted among formations with substantially different mineralogical compositions and porosities because these basic properties affect many other features and processes. The same is true for transfer of information among sites with very contrasting states of the system (e.g. porewater salinity, stress field). Overall, transferability is feasible at least to some degree among weakly to moderately consolidated formations. The fact that fracture flow and transport may occur in some highly compacted formations limits the transferability of findings from/to less compacted formations, as the dominant role of microstructure as a basis for transferability may no longer apply.

In the specific examples illustrating transfer of information among Opalinus Clay at Mont Terri, at Benken and the Callovo-Oxfordian at Bure, the basis of transferability for a number of transport-related and geomechanical features and processes is particularly good due the similarity of the mineralogical composition and of porosity. Differences in the states of the system exist but are well known and can be accounted for when transferring information. The transfer of information from natural analogues, as exemplified by the Jordanian limestone-hosted cementitious systems, is often restricted to a specific process or part of the system for which a basis of transferability can be demonstrated (e.g. the interaction of hyperalkaline water and rock matrix), while other features (e.g. the size and large-scale geometry of the hyperalkaline plume) are not transferable.

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GEOSCIENTIFIC DATA COLLECTION AND INTEGRATION FOR THE WASTE ISOLATION PILOT PLANT

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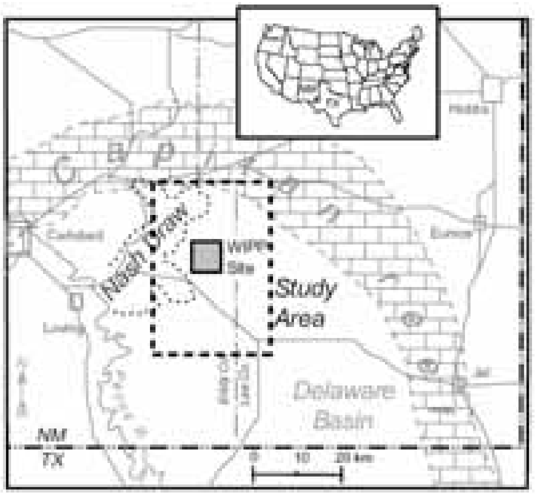
Introduction

Site characterisation for the Waste Isolation Pilot Plant (WIPP) (Figure 1) began with the drilling of the first borehole in 1974. Over the next two decades, site-characterisation activities included drilling, logging, and testing of over 100 boreholes, surface-based and borehole geophysical surveys, shaft and repository excavation and mapping, hydraulic testing in wells of formations above and below the repository host formation, hydraulic testing of the host formation in boreholes drilled from within the repository, hydrogeochemical sampling, geomechanical testing, and a host of geologic studies (sedimentology, mineralogy, petrology, deformation, dissolution, etc.). Integration of the information provided by these activities has yielded a robust understanding of the geologic setting of WIPP, but uncertainties remain with respect to the cause and distribution of fracturing in formations above and below the host formation. This paper describes recent efforts to identify relationships among various geoscientific properties, processes, and parameters to allow extrapolation of observed/measured conditions to less-characterised regions.

Figure 1. **Location of the WIPP site and principal study area.**



Data collection and integration

Different types of geoscientific data are integrated for different specific purposes. Most recently, many types of data have been integrated to develop, first, a new conceptual model of the hydrogeology of the Culebra Dolomite Member of the Rustler Formation [1, 2] and, second, a new numerical implementation of that model. The Culebra is the most transmissive unit overlying the repository (Figure 2), and the likely groundwater transport pathway for radionuclides released from the repository by future inadvertent human intrusion. The groundwater flow model for the original WIPP license application was based on kriging of the 44 transmissivity (T) measurements that had been made up to that time, with little soft geologic information included to explain the observed distribution of T or predict T's in untested areas. The Culebra hydrologic system was assumed to be at steady state, perturbed only by anthropogenic activities related to the characterisation of the site and construction of the repository. As the time for first re-licensing (required every five years) approached, on-going monitoring of water levels had shown that the Culebra is not at steady state, requiring a more comprehensive evaluation of both old and new data.

Geologic, core, and/or geophysical logs from approximately 500 boreholes were used to define stratigraphy and facies variations in the region surrounding the WIPP site [3]. Outcrops and shaft exposures were used to increase our sedimentologic understanding of lateral facies variations (Figure 3) and small-scale features observed in core [4, 5]. This allowed us to create a map (Figure 4) showing where halite (e.g. H4) is currently present in the non-dolomite members of the Rustler Formation, where mudstone (e.g. M4) rather than halite was deposited in these members, and where halite may have been dissolved [3]. By contouring the thicknesses of intervals between insoluble "marker" beds in the upper Salado, regions of gradual thinning most likely related to deposition could be distinguished from regions of rapid thinning most likely related to dissolution. This allowed definition of a margin delimiting the extent of upper Salado dissolution (Figure 4; [3]). Other maps were constructed showing Culebra structure contours and overburden thickness above the Culebra [3].

Figure 2. **WIPP stratigraphic column.**

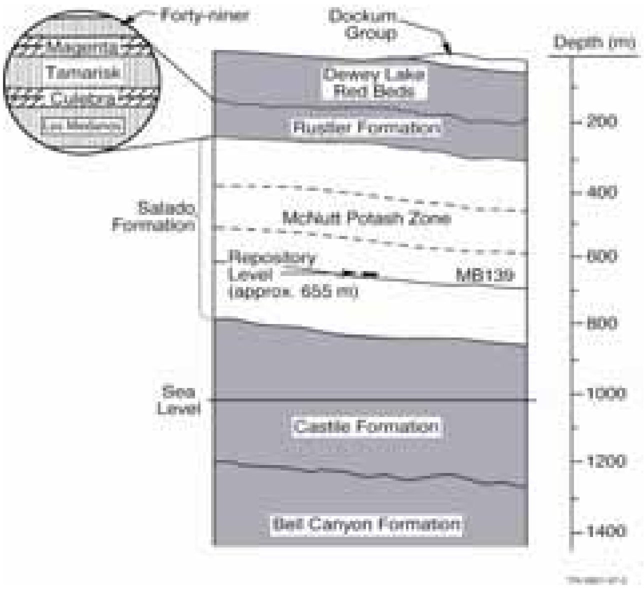


Figure 3. **Detailed stratigraphy of the Rustler Formation.**

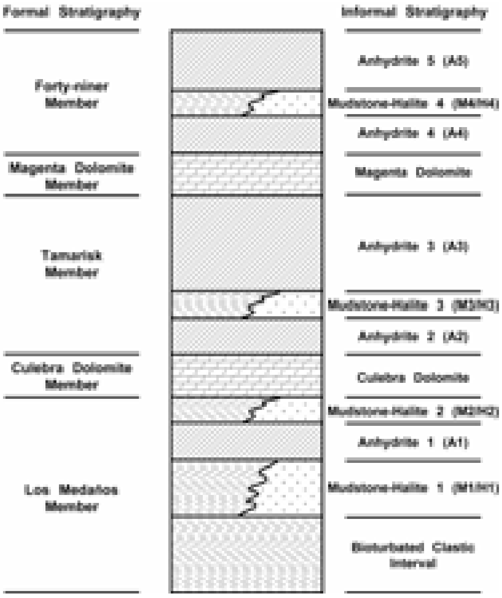
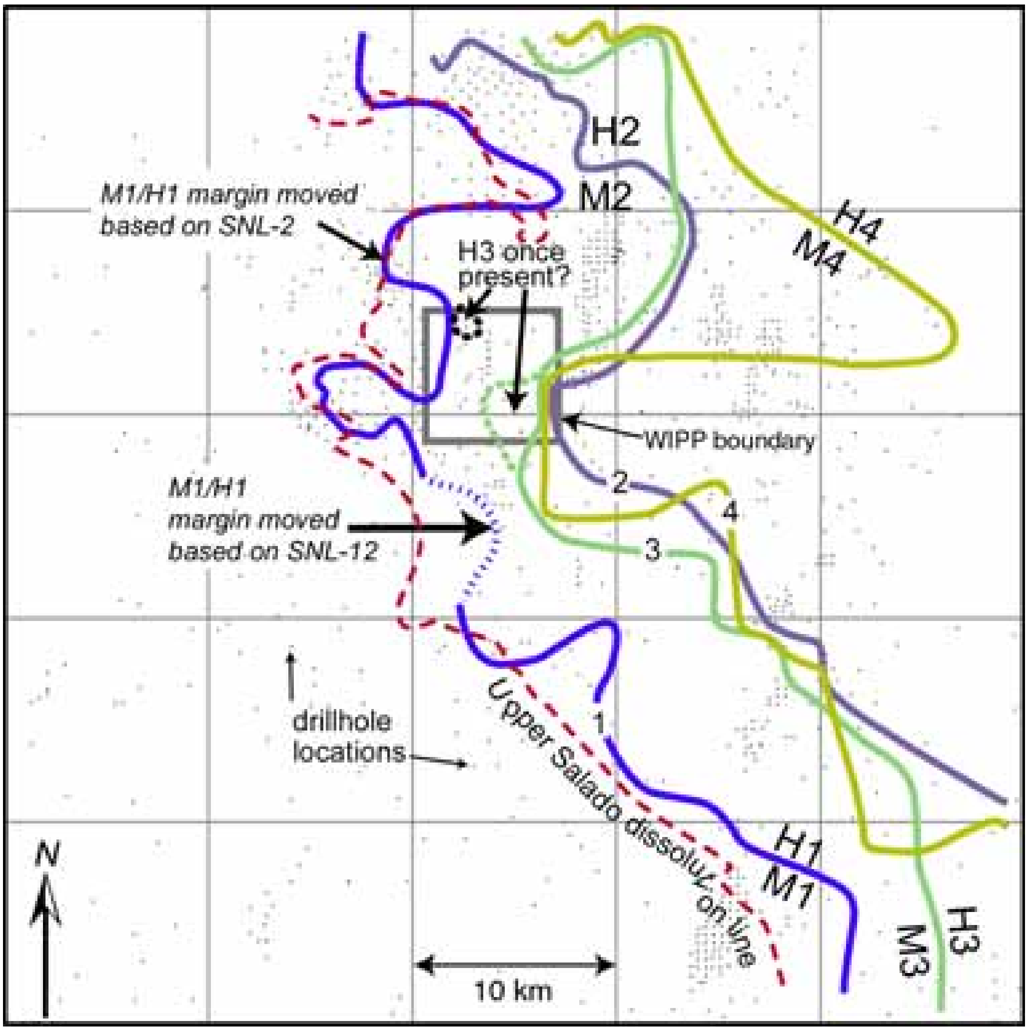
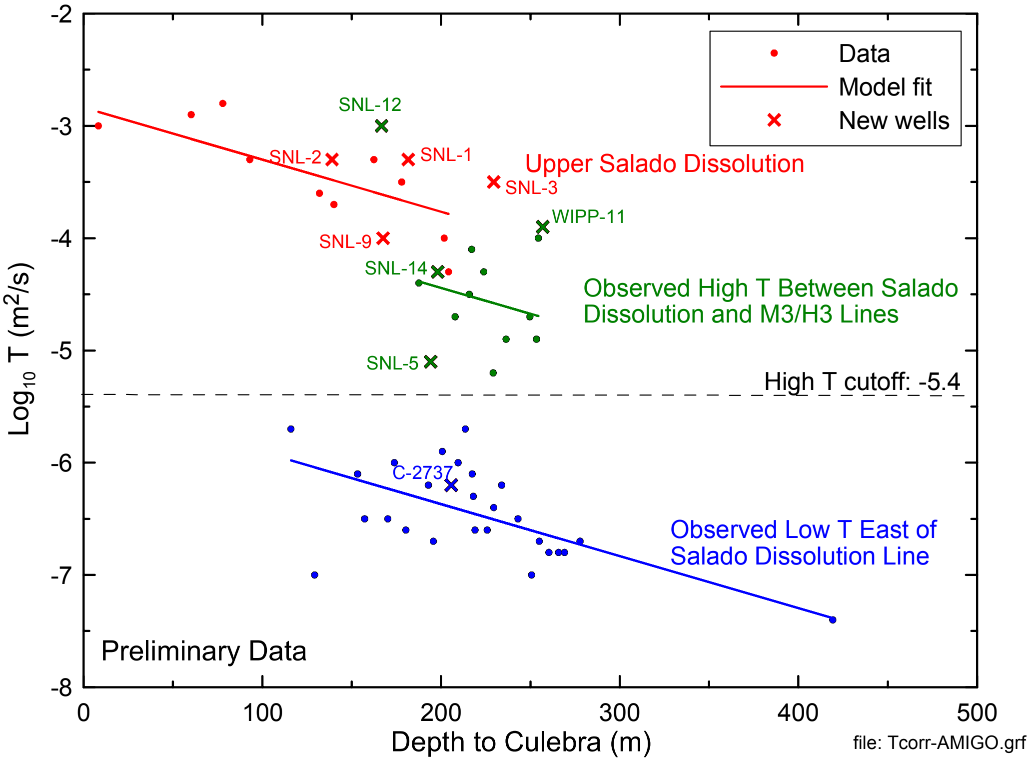


Figure 4. **Halite depositional margins in the Rustler Formation and Salado dissolution margin.**



Through 2003, transmissivity (T) estimates were available for the Culebra from hydraulic tests at 46 well locations. Plotting $\log_{10}$ T versus thickness of overburden above the Culebra, three groupings of data were observed (Figure 5; [6]). Two of these groupings could be related to geologic factors: the highest T's are observed where upper Salado dissolution has occurred, and the lowest T's are observed where halite is present above and/or immediately below the Culebra (M3/H3 and M2/H2 in Figure 3). The middle group of data represented wells showing moderately high T where no upper Salado dissolution has occurred and halite is present only in the lowermost Rustler (i.e. west of the M3/H3 and M2/H2 halite margins shown in Figure 4). We also observed that the hydraulic-test responses in the wells with moderately high to high T showed double-porosity effects indicative of fracturing, while the responses in the wells with low T were typical of a simple porous medium. Core and other borehole data also indicated that the Culebra is relatively unfractured at the low-T locations, and moderately to highly fractured at the higher T locations. Thus, the highest T's can be attributed to fracturing caused by dissolution of the upper Salado and subsidence of the Culebra, and the lowest T's reflect the absence of dissolution and subsidence. No testable hypothesis has been developed to date, however, to explain the moderately high T's where no upper Salado dissolution has occurred and halite is absent from the Rustler above M1/H1.

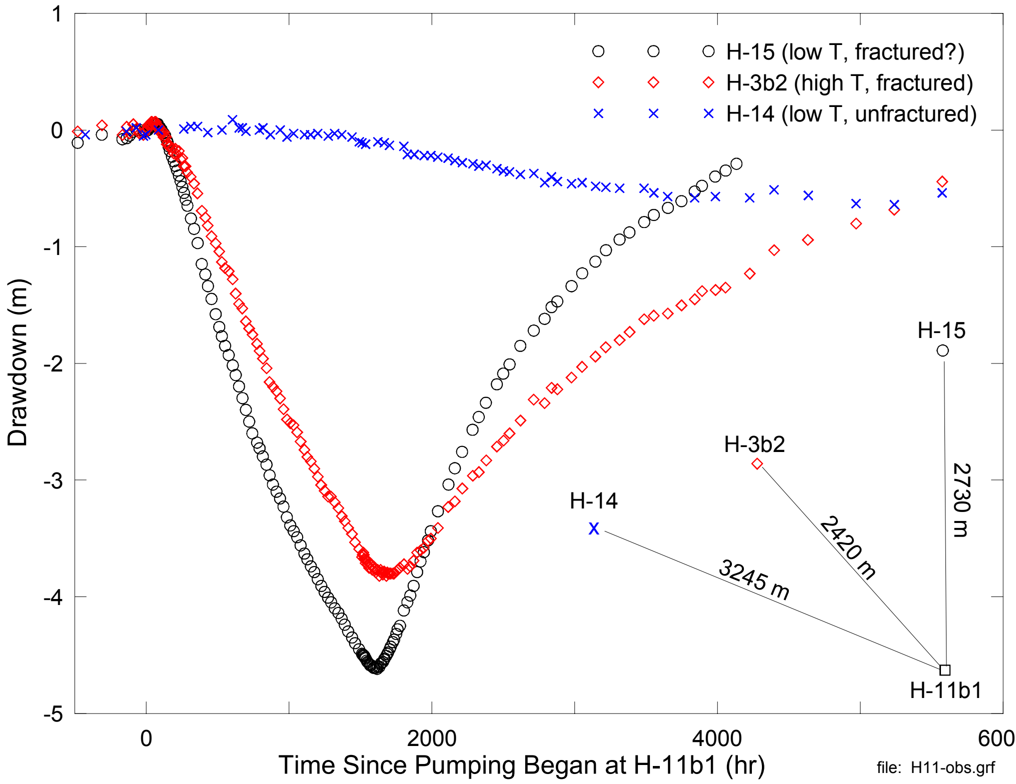
Figure 5. **Log_{10} Culebra T versus overburden thickness, with linear-regression fit.**



While the new conceptual and numerical models of the Culebra are plausible and consistent with the available data, our ability to use the maps and correlations to predict properties in areas lacking Culebra wells remained uncertain. Hence, a new well drilling and testing programme was initiated in 2003. To date, 13 new wells have been completed (nine of which have been tested so far), with five more wells planned to be drilled in 2006. Most of the new wells have encountered the conditions we expected (Figure 5), helping to substantiate our new conceptual model. However, we continue to be unable to predict whether we will encounter high or low T in the region between the Salado dissolution line and the M3/H3 halite line. No structural characteristics, geophysical log signatures, or known dissolution correlate with T in this region. The only tool that seems to be effective at defining where high T is or is not present in this region is large-scale pumping tests.

The patterns of pumping-induced responses observed in distant observation wells have proven to be reliable indicators of the presence or absence of fractures in particular regions, although precise locations of fractures cannot be defined. Observation wells that show rapid, high-magnitude responses to pumping must be close to, if not directly intersected by, fractures connected to the pumping well, regardless of the T measured in single-well tests (Figure 6). For instance, testing at well H-15 showed low T and no evidence of fracturing, but then H-15's response to pumping at well H-11b1 (shown in Figure 6) suggested that fractures must be near by. In the past year, three pumping tests of 22 to 32 days duration have been performed west, north, and south of the WIPP site to provide transient response data from observation wells up to 9.5 km from the pumping wells. Two-dimensional groundwater model calibration to the pumping-test responses provides the possibility of determining the most likely fracture locations, although the promise of this technique has yet to be fully realised in practice.

Figure 6. **Observation-well responses to pumping at H-11b1 showing presence and absence of fracture connections.**



Dealing with uncertainty

Uncertainty in the distribution of T within the Culebra affects modelling of groundwater flow and radionuclide transport through the Culebra for WIPP performance assessment. To deal with this uncertainty, a multi-step process was developed to generate and calibrate T fields for modelling. First, a single least-squares linear-regression fit was determined for all of the T data, with fixed offsets between the three groupings (Figure 5; [6]). By combining the regression equation with a map of overburden thickness, continuous distributions of Culebra T were developed for the regions where Salado dissolution has occurred and where halite is present in the Rustler above M1/H1, leaving just the middle region with undefined T's. To capture the uncertainty in this region, 100 different realisations of the T field were created using a stochastic process to assign either high or low T in areas lacking wells (Figure 7; [6]). Calibrating these "base" T fields to both steady-state heads and the transient heads associated with long-term pumping tests (Figure 8) then allowed us to develop a distribution of possible radionuclide transport paths (Figure 9) and travel times (Figure 10) from a point above the WIPP disposal rooms to the site boundary [7].

Figure 7. **Example base T field.**

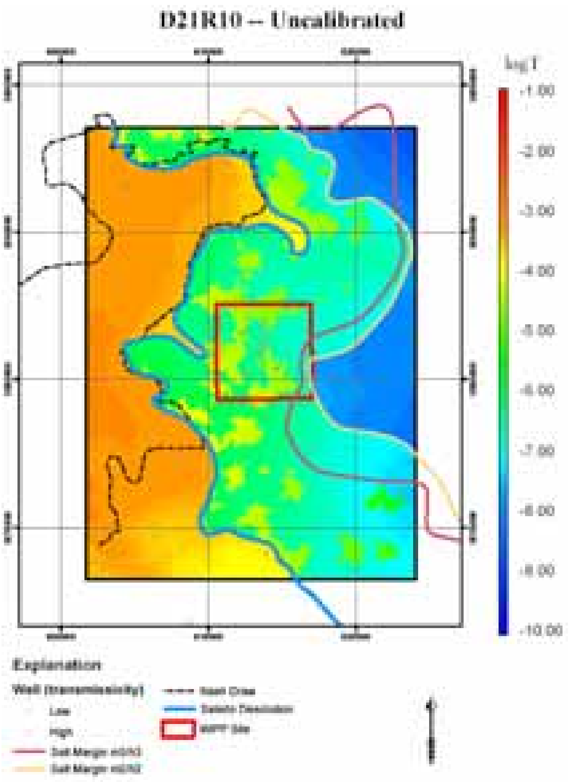


Figure 8. **Example calibrated T field.**

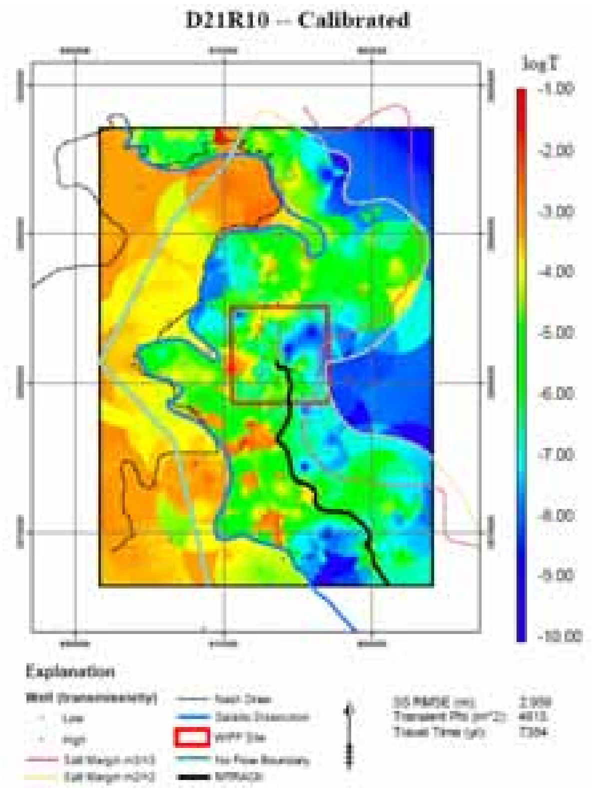


Figure 9. **Off-site travel paths through Culebra from particle tracking.**

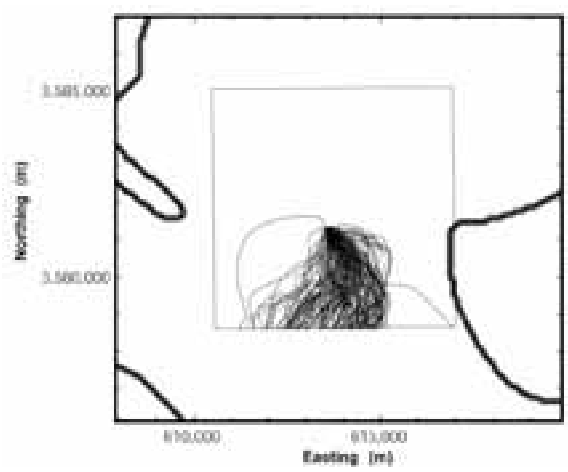
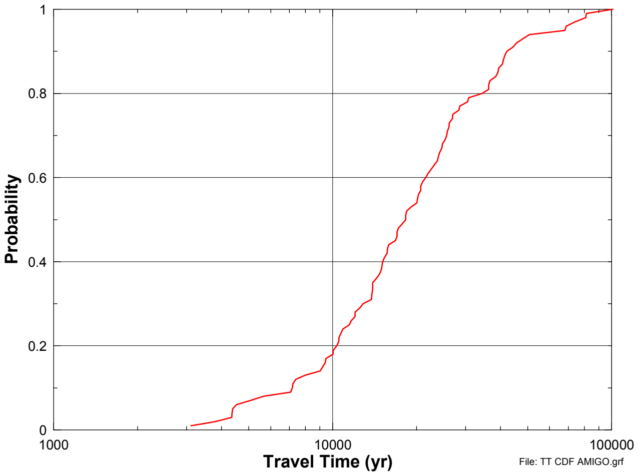
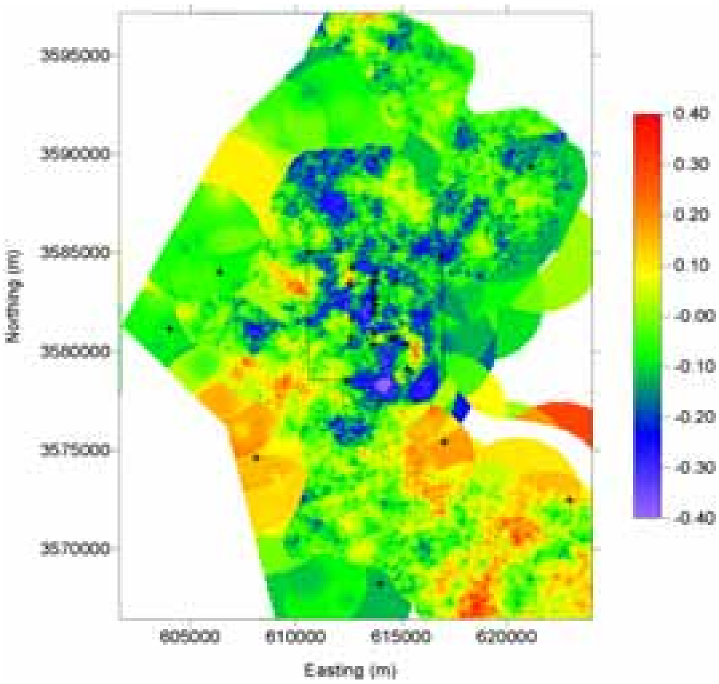


Figure 10. **CDF of off-site travel times for conservative solutes.**



Use of this type of probabilistic method allows us to bound the uncertainty in travel times associated with the uncertainty in fracturing. To reduce this uncertainty, we have used the calibrated T fields to identify the areas in the model domain where uncertainty in T has the largest effect on travel time (Figure 11; [8]). This sensitivity study has been used to guide the locations of new wells. Future versions of the model will incorporate measured T values at the most sensitive locations, reducing uncertainty.

Figure 11. **Rank correlation coefficient between calibrated T values and travel time to the WIPP boundary (well locations with inferred values of T shown by + symbols).**



Conclusions

Numerous types of geologic data from boreholes, well logs, and core have been combined with hydrologic measurements and observations to develop conceptual and numerical models of the distribution of transmissivity in the Culebra. Transmissivity extremes are found east and west of the WIPP site, and have well-understood geologic explanations. But no testable explanations exist for the localised occurrence of fracturing in areas where no dissolution of the upper Salado has occurred. Large-scale pumping tests have been performed to provide both information on the distribution of fractures and transient response data that can be used for model calibration. Uncertainty is addressed probabilistically by generating multiple realisations of the Culebra T field. Sensitivity studies performed on the calibrated T fields allow identification of the uncertain areas having the greatest effect on travel time, guiding the future installation and testing of wells.

A new drilling and testing programme has been initiated to test the hypotheses and correlations developed thus far, and to provide additional data for future modelling. A new generation of T fields will be developed for the next WIPP recertification application based on the improved conceptual model and recently collected data. A new evaluation of variations in Culebra brine compositions is also planned to allow us to eliminate T fields that predict flow directions that are inconsistent with observed water quality variations.

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Acknowledgements

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REVIEW OF A SITE DEVELOPER'S GEOSCIENTIFIC DATA AND SITE-CHARACTERISATION INFORMATION TO SUPPORT REPOSITORY CERTIFICATION

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Brief background

The Waste Isolation Pilot Plant (WIPP) in New Mexico is a first-of-a-kind deep geologic facility for the disposal of transuranic (TRU) radioactive waste from weapons production in the United States. In 1993, Congress authorised the Environmental Protection Agency (EPA) to develop and implement WIPP-site-specific compliance criteria based on the general safety and environmental standards in EPA's high-level and transuranic radioactive waste regulations [1]. EPA published its site-specific regulations [2] in 1996 and certified WIPP to open in 1998.

This regulatory framework set the stage for balancing diverse input data, provided a structure for document development, provided a mechanism for interaction between EPA and the Department of Energy (DOE), and provided a guide to support our review of WIPP's safety assessment. EPA's involvement continues during WIPP's operational phase.

Confidence in repository site geoscientific data enhances the regulator's ability to make a credible and defensible certification (licensing) decision and to communicate the basis for the decision to the public. Lack of confidence in the data can lead to lack of credibility about site suitability.

Balancing diverse input from various disciplines to synthesise lines of evidence

As the site developer, it was incumbent on the Department of Energy and its prime scientific adviser, Sandia National Laboratories (SNL), to develop the initial scientific basis for the site, such as the conceptual model of the disposal system. The bulk of this work occurred during the 1980s and into the early 1990s. The focus of EPA's initial review was to verify that the WIPP site was adequately characterised, had sufficient information about the site, was well documented, and supported DOE's conclusion that the WIPP repository would successfully contain radioactive waste. In addition, EPA had to ensure that any decision, especially one of approval, would be able to withstand a legal challenge in U.S. courts. Thus, the major influences in our decision-making process were technical considerations, public concerns, and legal considerations.

EPA was in the position of reviewing information from various sources, including DOE/SNL, the Environmental Evaluation Group (EEG, an oversight group in the state of New Mexico), the New Mexico Attorney General's office, National Academy of Sciences reports and information from their WIPP meetings, EPA-required peer reviews, and comments from the general public. An example of how we balanced diverse input is in our review of DOE's model selection, both computer and conceptual. We realised that there could be different approaches to identifying a specific computer model or process that should be used by DOE. This was especially pronounced in the selection of computer models and the quest to identify the "best" computer model for a particular phenomenon. EPA came to the conclusion that if the model adequately addressed the issue, was adequately documented and tested for its use, then it could be used. An additional aspect of concern was how the model was used. If DOE could show that a certain approach (e.g. parameter selection) was conservative (i.e. it predicted more releases than another approach), then we could more readily accept the approach. If there were multiple conceptual models that could be used to adequately explain a certain phenomenon, then DOE usually decided to use the more conservative one.

Central to our review process was the prioritisation of the most important issues such as: features, events, processes (FEPs); resulting scenarios; and important parameters. DOE's scenario identification process narrowed the initial list of important issues and DOE's multiple performance assessments and additional modelling further identified the important FEPs and parameters. A key part of this was DOE's use of "sidebar calculations" with which DOE conducted analyses of the effect of different processes on some important metric, such as gas generation. Additional EPA-led sensitivity analyses, separate from DOE's analyses, also provided information about parameter importance. EPA also conducted some independent analyses to understand the effect of certain processes, such as groundwater flow and radionuclide transport. The combination of our analyses and a review of DOE's analyses helped us narrow the important FEPs and parameters.

Specific regulatory requirements were the tools we used to balance diverse input and to ensure that DOE's activities were done well, complete, and supported the safety case. The general safety and environmental standards in 40 CFR 191 [1] specify general requirements and standards that DOE was to meet. 40 CFR 194 [2] describes site-specific requirements that DOE had to meet to provide adequate data, complete documentation, and verification of data quality used to support the safety determination. These requirements also apply to the periodic re-certifications that WIPP must undergo.

From our experience in reviewing data from WIPP, we have identified questions that need to be addressed when balancing information from diverse disciplines. These include:

- Is there enough information to make a determination?
  - Has the repository developer identified the major processes that could affect safety?
  - Do the data reflect the expected major processes or are there important data gaps?
  - Is there confidence that the supporting information is usable, traceable, and technically – and legally defensible?
  - Can the modelling system reasonably represent the major elements of the disposal system, both natural and engineered?
  - Is there agreement that the conceptual models generally reflect what is expected to happen at the disposal site?
  - Do the computer codes implement the conceptual models so that there is confidence in the results?
  - Can the repository developer's results be reproduced?
  - Do independent peers agree with the conceptualisation of the disposal system?

- To what extent can the characteristics of the site provide a barrier to radionuclide migration?
  - The site suitability question must first address the issue of whether the site geology performs as a barrier. Assuming there were to be no significant engineered barriers at the site, what would happen to the waste under base-case conditions or the higher precipitation case – for example?

Regulatory guidance for structuring documentation

EPA set very specific requirements for the WIPP in 40 CFR 194 [2] and our Compliance Application Guidance [3] related to acceptable site-characterisation data and data used to support all aspects of the safety assessment. We required a description of conceptual models and scenario construction and that they must represent reasonable future states of the disposal system, include a description of alternative conceptual models, that computer numerical schemes obtain stable solutions, computer models produce accurate results, that conceptual models are peer reviewed, that all work is done using a national standard quality assurance framework, and many more specific requirements. In the flowchart below (Figure 1), we identify the sections of 40 CFR 194 that correspond to different activities, such as site characterisation and performance assessment. Many of these sections have some documentation requirement.

An issue that was of concern to us was getting appropriate and complete documentation for the modelling and computer codes. Specific requirements in the models and computer codes and quality assurance sections were crucial in our obtaining the documents that we needed to complete our review. In spite of the regulatory requirements, it sometimes required upper management intervention for EPA to get the needed documentation from DOE or SNL.

EPA's regulation required that parameters be documented and be based on data or else DOE would have to use an expert judgment[1] process to establish the parameter. In our review, we identified that one important WIPP parameter, particle diameter of materials to be released up a human intruded borehole, had no supporting data and therefore needed an expert judgment panel.

Requirements of 40 CFR 194 provide the framework for complete documentation and our Compliance Application Guidance [3] (CAG) documents EPA's specific documentation and data quality expectations. For example, these regulations require DOE to provide: "Detailed descriptions of data collection procedures, sources of data, data reduction and analysis, and code input parameter development…" for all aspects of the WIPP, such as site characterisation and result activities. In section 22 of 40 CFR 194 [2], EPA required DOE to implement a rigorous quality assurance (QA) programme at WIPP. QA requires very stringent demands for all data and documentation that support site characterisation and safety assessment activities, such as safety (performance) assessment calculations. Also, our QA requirements provide the tools to assure that the documentation produced by DOE was complete and as accurate as possible. For example, NQA [4] requires very specific documentation be developed to support data or computer codes used in the safety assessment. These include a Requirements Document, Validation and Verification Document, Implementation Document, and a User's Manual. While QA requirements aim to ensure that activities are "doing the right thing right," we used the QA documentation, such as the User's Manuals, to help us determine if DOE was "doing the right things."

As part of EPA's compliance criteria, DOE also was required to have formal independent peer review of several topics, including conceptual models. DOE had additional reviews conducted by the National Academy of Sciences (NAS) [5]. Their final report came before EPA's decision and provided additional review of DOE's analyses. The NAS positive recommendation gave added confidence to EPA's decision.

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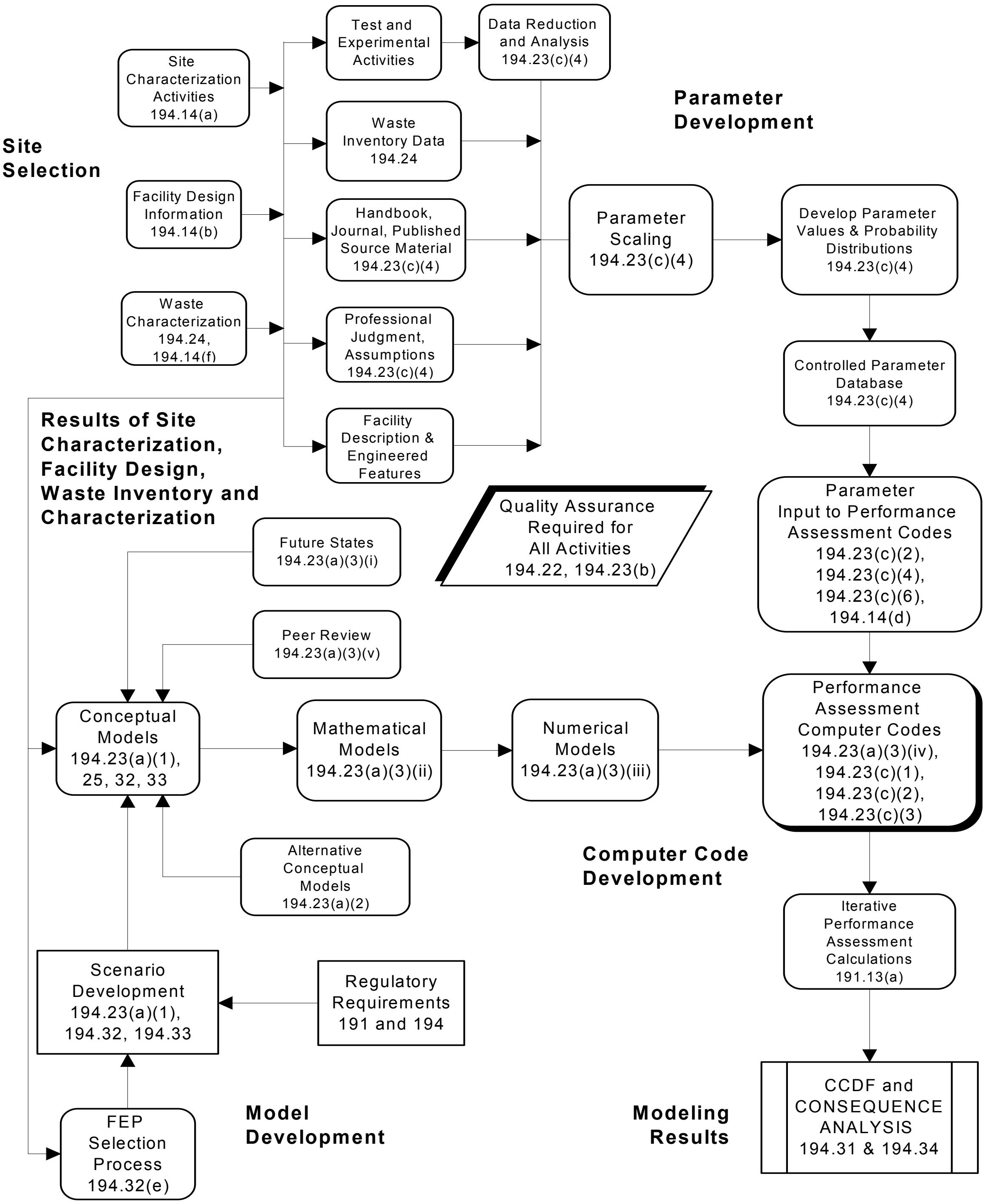
[1] Expert judgment should not be confused with professional judgment. We consider professional judgment as what is used when interpreting data. Expert judgment is used when there are no data.

Figure 1. **Flowchart of important repository characterisation steps and associated sections of 40 CFR 191 and 40 CFR 194. These are grouped according to major activities, such as site selection and parameter development.**



Needs and mechanisms for interaction between the regulator and implementer during site characterisation

EPA interacted with DOE on both a formal and informal basis. Much of the time we were able to interact informally with DOE and DOE's contractors via phone or meetings with individuals. When our office was working on regulations, our interactions with DOE were guided by a formal process with set requirements, such as documenting conversations and using public meetings. Formal "technical meetings" were used on some topics and were typically overview types of presentations that gave the public a chance to participate in the review as it unfolded. EPA and EPA contractors also met with DOE, SNL and other DOE contractors frequently during the site approval process.

A large part of our activities involved understanding what DOE and its contractors were trying to do and had done during site characterisation. We also provided guidance on the type of analyses or documentation that was required. When we began working on the WIPP project, we focused on understanding the issues and DOE's approach. Once familiar with the project, we began to identify needs and raise concerns. Finally, we needed to make judgments for the certification (license) decision.

A strong working relationship between the regulator and implementer, both during site characterisation and during the development and operation of the facility, is critical to success of any repository programme. Regulations should specify the nature and scope of these interactions, both formal and informal, in well-written clear and specific regulations. The interactions can be significantly enhanced by constructive staff-to-staff cooperation.

Processes to deal with issue resolution between regulator and implementer

EPA's requirements are laid out in the regulations and the focus is on ensuring requirements are met. During the course of our review, we would need to get information from DOE. Many times we could get issues resolved at the staff level. However, there were situations where issues needed to be elevated. This occurred for different reasons, such as the interpretation by DOE or the scientists that something was not necessary for EPA to have. Correspondence from EPA to DOE mid-level management was typically sufficient to address the issues. In the cases where this correspondence did not work, higher-level management addressed the issue. The key in this process for the regulator is that the implementer must have a positive response from the regulator.

Overall this staff-to-staff approach worked effectively on the WIPP project. Seldom was management included to resolve issues during the original site approval process. Management involvement actually did enhance the efficiency of our process. Problems were solved and the project was able to continue with few obstacles that blocked progress of our work.

Ensuring that the documentation supports the needs of the scientific community reviewing the safety assessment

In our view, this is related to regulatory guidance for structuring documentation. In the case of WIPP, we required extensive documentation in many areas (see Figure 1). However, EPA's involvement came after much of the site-characterisation data had been collected. In order to be able to support EPA's documentation requirements, DOE had to rely on peer-reviewed journal documentation and internal documentation that underwent some form of peer review. To their credit, DOE convened an ongoing (at that time) scientific oversight subcommittee of the U.S. National Academy of Sciences which raised numerous scientific issues. An additional group, the Environmental Evaluation Group, was also instrumental in raising issues of concern. In our opinion, having information published in the public domain is important, but formalised external groups are also essential.

Conclusion

Clear regulations and specific quality standards can enhance the quality of site-characterisation documentation and assist the regulator in its approval process of the site. In EPA's regulations, documentation is required on numerous issues, and EPA supplemented this with guidance. High-quality documentation is essential, especially for EPA. In the certification process for WIPP, the documentation in the record and our written interpretation of the record was what was used in legal proceedings that followed EPA's certification of WIPP.

EPA and DOE had frequent and generally open communication. During formal regulatory proceedings, all communication had to be documented. Some decisions were made at the staff level, but major decisions were typically addressed and resolved through correspondence.

DOE was able to demonstrate, primarily through its documentation, that the WIPP site would comply with EPA's regulations and numerical release standards. The same documentation, plus additional documentation EPA felt was necessary for a decision, formed the basis of a certification decision that withstood legal challenge. The combination of good documentation, open communication between the regulator and implementer, and resolution of issues are all important in developing confidence that a site is suitable. An important aspect of the process, however, is that the implementer can show that the site will contain the radioactive materials.

Some recommendations

- The regulator can use regulatory requirements to direct the site developer to produce high-quality documentation of site-characterisation activities and results found in the safety assessment calculations.

- Regulations need to identify the documentation needed so that the regulator can defend its decision. Implementers need to provide documentation required by the regulator. The answer to "When is it enough?" can be determined by when the regulator believes that there is enough that it can defend a decision.

- The implementer and regulator staffs need to strive to work as effectively as possible. Problems that arise should be discussed, resolved, and clearly documented.

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ASME NQA-3-1989 edition, "Quality Assurance Programme Requirements for the Collection of Scientific and Technical Information for Site Characterisation of High-Level Nuclear Waste Repositories" [excluding section 2.1(b) and (c)].

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GEOLOGICAL STORAGE OF CO_2 AT THE WEYBURN OIL FIELD, SASKATCHEWAN: SUMMARY OF RESULTS OF THE IEA GHG WEYBURN CO_2 MONITORING AND STORAGE PROJECT

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1. Introduction

The IEA GHG (International Energy Agency, Greenhouse Gas R&D Programme) Weyburn CO_2 Monitoring and Storage Project was initiated to study the potential for geological storage of CO_2 in a depleting oil field in southeastern Saskatchewan, Canada. In October 2000, EnCana Resources (at that time PanCanadian Energy) began an enhanced oil recovery (EOR) project involving the injection of anthropogenic CO_2 into Mississippian carbonates of the north eastern Williston Basin. The goal of the EOR operations is to recover an additional 20.7 x 10 ^{6} m^3 (130 x 10^6 bbls) oil which will extend the life of the Weyburn Oil Field by at least 25 years. About 5 000 tonnes/day (3 x 10^6 m^3) CO_2, purchased from Dakota Gasification Company's Great Plains Synfuels Plant in Beulah, ND, are transported via pipeline 320 km to the Weyburn Field. The CO_2 is greater than 95% pure and is injected into the reservoir as a supercritical fluid where it reduces the viscosity of the residual oil through miscible mixing thereby improving ultimate hydrocarbon recovery. The Weyburn Project, coordinated through the Petroleum Technology Research Centre in Regina, Saskatchewan, developed a research programme to accompany EnCana's EOR project to investigate CO_2 in the subsurface to 1) determine the potential of the reservoir to serve as a container for long-term (ca. 5 000 years) storage of the anthropogenic CO_2, 2) enhance the effectiveness of the miscible flood for EOR, and 3) to determine the economic feasibility of long-term storage. Phase 1 of the Weyburn Project began in July 2000 and was completed in September 2004.

Investigations involved in the Weyburn Project were multidisciplinary and required grouping into eight Principal Tasks which included more than 70 Subtasks. The Principal Tasks include: field-based programmes jointly funded by EnCana and the Weyburn Project; Geoscience Framework; Geochemical Modelling; Geophysical Monitoring; CO_2 Storage Performance; Storage Economics; Project Control; and European Commission Studies. More than 20 million dollars funding for the project was provided by fifteen sponsors including Natural Resources Canada, United States Department of Energy, Saskatchewan Industry and Resources (SIR), Alberta Energy Research Institute, the European Community and ten industrial sponsors in Canada, the United States and Japan. More than 20 research and consulting organisations performed research within this study and provided additional in-kind support worth 20 million dollars.

The results of the project were ultimately grouped into four major themes: Geological Characterisation; Prediction, Monitoring, and Verification of CO_2 Movements; CO_2 Storage Capacity and Distribution Predictions and Application of Economic Limits; and Long-Term Risk Assessment of the Storage Sites. This abstract will focus mainly on the Geological Characterisation Theme and briefly summarise its findings.

2. Geological characterisation

2.1 *Scope of investigation*

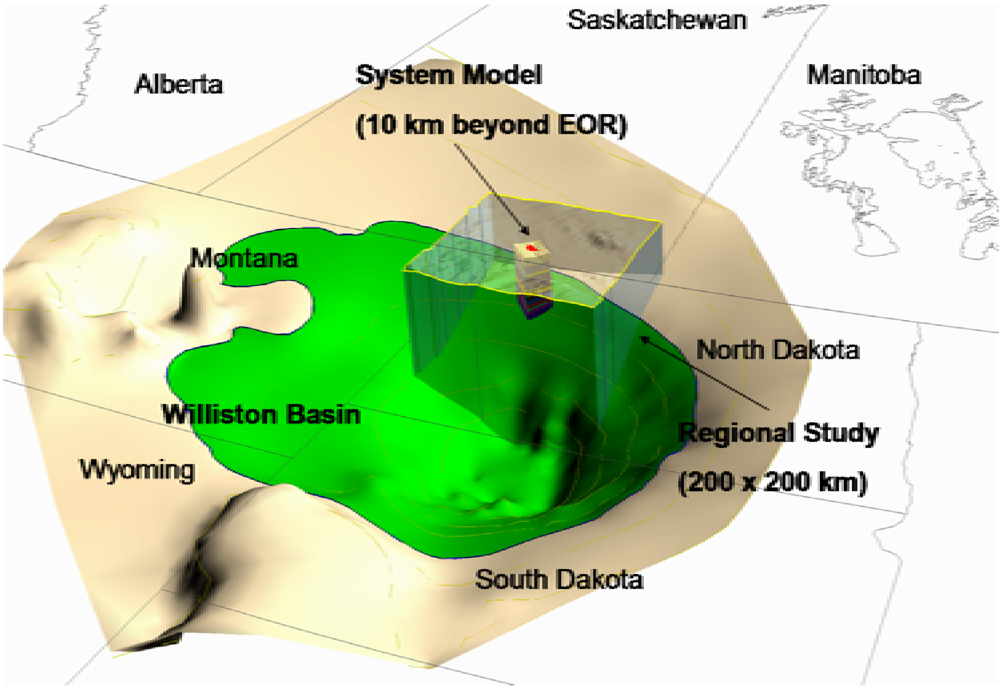
Geological characterisation was one of the largest and most diverse aspects of the Weyburn Project. The overall goal was to evaluate the geological integrity of the Weyburn Oil Pool and the surrounding geosphere for storing injected CO_2 for hundreds to thousands of years. This involved providing a regional framework in which other, more detailed, studies may be placed. Regional geological mapping was performed throughout the entire Phanerozoic succession from the Precambrian basement to ground surface, a thickness ranging from 2.5 to over 4 km, across a region 200 x 200 km centred on the Weyburn Field (Haidl *et al.* in press). This area included much of the northern Williston Basin including southeastern Saskatchewan and portions of north western North Dakota and north eastern Montana (Figure 1). Approximately 2 000 km of pre-existing regional 2-D seismic data within this region were re-processed to identify the distribution of faults and fractures within the system. High Resolution Aeromagnetic data (HRAM) greatly aided in establishing a 3-D network of regional fault and subsurface tectonic lineations. Detailed surface examination of lineament patterns using airphoto and satellite imagery was performed to determine whether subtle surface features may reflect vertically translated expressions of subsurface structures.

Within the regional study, a detailed hydrogeological study of the bedrock aquifers (and aquitards) was undertaken to determine controls over subsurface fluid movements including rates, directions and other physicochemical characteristics (Khan and Rostron, in press). Shallower hydrogeological studies were performed across the area to identify potable and agricultural water sources in Upper Cretaceous, Tertiary and Quaternary strata. A smaller area was also targeted to develop a detailed geological, or system, model for use in numerical simulations and risk assessments of subsurface CO_2 movement and storage. This area extended about 10 km beyond the limits of the EOR region (see Figure 1). Within this focused area, detailed shallow hydrogeological mapping was performed including a side-project to delineate more precisely a shallow aquifer that potentially contained potable water near the Weyburn Field. Additional stochastic simulations using the deep hydrogeological data such as permeability and water chemistry of specific aquifers was performed to provide additional information on fluid and rock characteristics for this region. Till samples were collected near the oil field to assist in the interpretation of soil-gas monitoring studies performed as part of the monitoring aspect of the project (White *et al.* 2004). Detailed geological mapping was performed of select units including evaporate layers in the Midale and Frobisher beds that serve as the top and bottom reservoir seals, respectively, and on the Lower Watrous redbeds, Colorado Group strata and the sequence stratigraphy of the Mississippian System in the Williston Basin. More detailed descriptions of the individual research studies within the Geoscience Framework portion of the Weyburn Project are provided in Whittaker and Gilboy (2003), Whittaker (2004) and Whittaker *et al.* (2002 and 2004).

2.2 *Results*

The Weyburn reservoir, in the Midale Beds of the Mississippian Charles Formation, is at an average depth of 1.5 km and includes an upper dolostone unit, the Marly, with an average thickness of about 6 m, and a lower limestone unit, the Vuggy, that averages around 15 m in thickness (Burrowes, 2001). The Vuggy contains porous grainstones developed along a carbonate shoal which form good-quality reservoir, and low porosity mudstones, interpreted to represent intershoal deposits that are of poor reservoir quality. Most oil production from the Weyburn Pool prior to the CO_2-miscible flood was from the Vuggy shoal regions. CO_2 is currently being injected into the Marly dolostones to access residual oil, although the CO_2 is moving through both the Marly and Vuggy. The upper seals to the reservoir are the Midale Evaporite, a highly competent sedimentary anhydrite layer ranging in thickness from one to more than 10 m, and a diagenetic zone in which Midale carbonates have been extensively altered and anhydritised resulting in virtually complete porosity occlusion. This diagenetically altered zone occurs at the up-dip portion of the Midale Beds immediately subjacent the regional Sub-Mesozoic Unconformity. The paragenetic sequence of diagenetic products and processes indicate that no recognisable fluid migration events have affected the altered unit post hydrocarbon emplacement approximately 50 to 55 Ma. Above the Sub-Mesozoic Unconformity are relatively impermeable beds of the Triassic Lower Watrous Member that serve as a regionally extensive aquitard across much of southern Saskatchewan. In fact the shaly, anhydritic siltstones of the Lower Watrous Member, or redbeds, arguably form the most important trap for hydrocarbon accumulation in the northern Williston Basin. The Watrous redbeds separate a deep hydrogeological system, which includes the Midale reservoir and essentially all Paleozoic strata, from intermediate and shallow hydrogeological systems. Intermediate (around 1 000 to 300 m depth) and shallow systems are much less saline, have higher permeabilities and faster flowing formation waters than the deep hydrogeological system. Total dissolved solids and pressure data indicate no evidence for flow across the Lower Watrous Member between the deep and intermediate systems; thus, the Midale Beds are effectively hydraulically isolated from shallower strata. The Watrous aquitard, therefore, is an excellent regional seal for CO_2 injected into the Midale Beds. The Midale aquifer has low flow velocities (<1 m/yr) and mainly horizontally oriented flow which favours hydrodynamic trapping of CO_2 thereby reducing the effectiveness of formation-water acting as a transport agent for CO_2. The geological setting of the Weyburn Pool is within a tectonically quiescent region. Although large-scale regional fractures and faults are present in the larger region, most faults observed are mainly localised disturbances without recognisable offset. Regionally extensive faults that may occur within the vicinity of the Weyburn Pool also exhibit limited offset and have not compromised hydrocarbon retention for the past 50 million years. Therefore, such faults are considered to be closed and likely do not represent fast pathways for CO_2 movement within the subsurface.

Figure 1 **Diagram of the region in central North America investigated as part of the Weyburn CO_2 Project. A regional geological framework was constructed for a 200 x 200 km area as depicted by the translucent outline. A more detailed system model was constructed for the region within 10 km surrounding the CO_2-flood.**

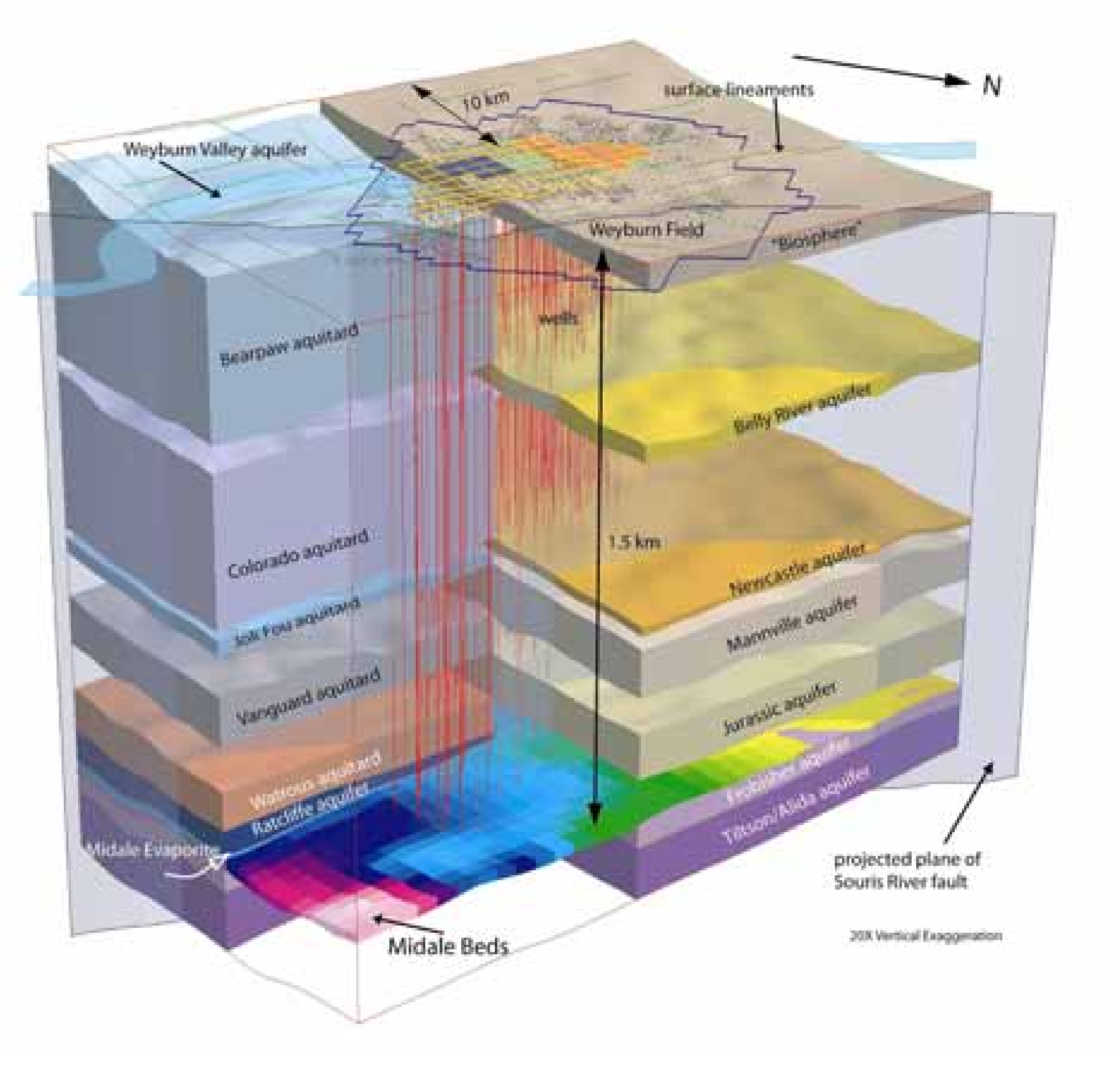


A detailed 3D geological model was constructed using the data obtained from the above studies. This model includes the geometry of the geological formations grouped into hydrostratigraphic units. Each hydrostratigraphic unit represents a rock package that acts mainly as an aquifer or as an aquitard (Figure 2). In the model, the units are populated with data such as porosity, permeability, salinity, temperature, pressure and additional information where available. Also included in the model is a projected fault plane, the Souris Valley Fault, identified in this study. The depth of the model extends from ground surface to the base of the Tilston Beds (about 200 m below the Midale reservoir), and the areal extent is 10 km beyond the limits of the CO_2 flood as described previously. This model served as the foundation for detailed numerical risk and performance assessment of long-term storage potential. Although currently no formal consensus exists on the timescale of long-term storage of greenhouse gases, 5 000 years is generally considered reasonable and was used in this study. Stratigraphic relationships and depositional and structural history of the basin also provided input into scenario and FEP development.

Results involving numerical reservoir simulation and history matching indicate that approximately 23 million tonnes (MT) CO_2 will remain in the reservoir at the expected end of EOR operations in 2033 (Law *et al*. 2004). This is determined considering only the 75 patterns currently planned for EOR that involves only the western portion of the Weyburn Field. The driving force behind the EOR project is, of course, to recover additional oil. Were CO_2 injection to be continued after the cessation of EOR operations to maximise CO_2 storage, however, it may be possible to store almost 55 MT CO_2 in the Weyburn reservoir (again, considering only the 75 pattern area). Both probabilistic and deterministic methods were applied to the Weyburn data to assess the fate of injected CO_2. Probabilistic risk and performance assessment modelling using numerical flow simulators to determine the long-term fate of the injected CO_2 indicates that no CO_2 will migrate above the caprock (i.e. Midale Evaporite) in 5 000 years (Chalaturnyk *et al*. 2004). Numerical modelling of risk and performance of long-term subsurface storage of CO_2 is still in its early stages of refinement and the Weyburn results are among the first ever to be determined relative to an actual injection site using real field data. Future work will focus on enhancing the resolution of the geological model and improving methods of risk assessment as applied to subsurface storage of CO_2. It is noteworthy, however, that these first results are supported by the geological investigations that also indicate that the Weyburn Pool is a suitable and secure location for the long-term subsurface storage of CO_2.

Of further support to the secure storage of CO_2 in geological media is that natural accumulations of CO_2 are found in very similar reservoirs to that at Weyburn approximately 400 km west along the western margin of the Williston Basin. Alkalic Tertiary intrusions into Paleozoic carbonates in the vicinity of the Little Rocky Mountains and Bearspaw Mountains of Montana about 50 Ma likely generated CO_2 that subsequently migrated approximately 100 km north. This CO_2 was trapped in Devonian strata comprised of thin carbonate cycles capped by evaporite beds formed in similar environments as the Mississippian rocks at Weyburn. The natural CO_2 reservoirs are found at depths of 1 600 to 2 000 m and are overlain by essentially the same geological package as that which occurs at Weyburn. The naturally occurring CO_2 has resided in these reservoirs for tens of millions of years, thereby suggesting that appropriate site selection can result in secure, long-term geological storage of greenhouse gases.

Figure 2. **Cutaway block diagram of the geological model developed for the Weyburn Project. The model depicts the major hydrostratigraphic units; on the left are aquitards and on the right are aquifers. The yellow grid on the ground surface indicates the area planned for CO_2 injection. Lineaments identified from satellite images and airphotos are presented as green lines on the surface, and the location of the shallow Weyburn Valley aquifer is also shown. The colour variations in the Midale Beds represent variations in salinity within this aquifer. All layers in the model are similarly populated with various property data. The plane of the Souris Valley Fault is shown for reference. The System Model used in risk assessment contains information regarding anthropogenic features such as wells, and pressure and fluid distribution related to oil-production methods.**



3. Summary

Detailed geological characterisation was performed to assess the geosphere encompassing the Weyburn Pool area regarding its suitability for long-term geological storage of CO_2. The characterisation included regional and detailed geological mapping, hydrogeological studies, regional geophysical investigations including seismic and HRAM, and remotely sensed imagery studies. A detailed 3D geological model was constructed from much of these data for use in numerical risk and performance assessment. The results from these and other studies conducted as part of the IEA Weyburn Project indicate that up to 23 MT CO_2 will remain in the reservoir at the end of EOR operations and that this CO_2, which otherwise would be vented to atmosphere, will remain securely stored within the geosphere for more than 5 000 years. Investigations into the geological characterisation of the region and numerical modelling have indicated that the Weyburn Pool is a highly suitable location for long-term geological storage of CO_2.

A second phase to the Weyburn Project is currently underway. In this next stage, considerable focus will be placed on improving the resolution of geological models and the tailoring of risk assessment techniques as applied to geological storage of CO_2. Additional areas of investigation of interest to geological characterisation include the potential movement of fluids along fractures and faults, petrophysical characterisation of shales as barriers to flow, and expanded use of geostatistical methods of populating regional geological models.

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CURRENT STATUS OF THE OECD/NEA PROJECT ON “NATURAL TRACER PROFILES ACROSS ARGILLACEOUS FORMATIONS” (CLAYTRAC)

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Introduction

Hydrogeological and geochemical investigations of clay-rich sedimentary formations in variable states of induration have recently been conducted or are underway. At several sites, data sets on the spatial distribution of natural tracer concentrations and isotopic ratios in matrix pore waters are available (anions, water isotopes, noble gases). Regular, curved profiles were observed for some tracers in some formations but are absent in others. Some tracer distributions have been interpreted as diffusion profiles (see, e.g. Patriarche 2004a,b for Tournemire/France and Gimmi & Waber 2004 for Benken/Switzerland).

Tracer profiles in argillaceous rock formations can be considered as large-scale and long-term natural experiments by which the transport properties can be constrained. They provide complementary information to that obtained from experiments in laboratories or underground facilities, where typical spatial scales are 1 cm to 1 m and temporal scales only rarely exceed 1 a. Natural tracer profiles can bridge the gap between these scales and those required for performance assessment (where typical scales are tens to hundreds of m and 0.1-1 Ma) and provide an independent line of evidence for system understanding as well as for safety considerations in qualitative and quantitative terms. Specifically, studies targeted at the interpretation of tracer profiles are useful for the upscaling of laboratory experiments.

The degree to which the evidence based on tracer profiles has been exploited to date is quite heterogeneous among sites and formations. Some of the techniques for measuring tracer contents have only been developed in recent years, and thus the quality of the available data is mixed. However, data sets obtained in the pioneering years can often be adjusted/corrected to represent current state-of-the-art knowledge.

Objectives of CLAYTRAC

CLAYTRAC (“Natural tracer profiles across argillaceous formations - review and synthesis”) is a project launched by the OECD/NEA Clay Club, running from January 2005 to December 2006. It is funded by Andra (France), BGR (Germany), IRSN (France), Nagra (Switzerland), Numo (Japan), Ondraf/Niras & SCK•CEN (Belgium) and Puram & Mecsek Ore Environment (Hungary) and is also supported by the OECD Nuclear Energy Agency.

The project does not include the collection of new data but is focussed on the re-evaluation of existing matrix pore fluid measurements and on evidence documented in the literature regarding formation-specific palaeo-hydrogeological evolution. The added value of the work compared to studies dealing with individual sites in isolation lies in the comparison and integration of data, results and conclusions from a variety of sites and formations. The application of a consistent methodology of data collection, processing and modelling is expected to meet the following objectives:

- To provide an overview of available data sets.
- To develop and apply a consistent way of data processing and evaluation that is the basis for comparability (e.g. consideration of tracer-specific porosities and diffusion coefficients).
- To evaluate the strengths and weaknesses of different tracers for quantitative understanding of transport processes in argillaceous rocks.
- To comment on commonalties and differences among the sites under consideration.
- To identify gaps in existing data sets and make recommendations for future data acquisition campaigns.

The observed spatial distributions of tracers are compared to numerical model calculations based on a variety of parameter sets and conceptual assumptions. Modelling efforts have the following objectives:

- To test the hypothesis that tracer profiles are consistent with diffusion as the dominant transport process.
- To place upper bounds on advective velocities across the argillaceous formation.
- To constrain the spectrum of initial and boundary conditions (based on the shapes of the tracer profiles).
- To compare and integrate the interpretations based on different tracers at any given site (site-specific consistency check).
- To compare and integrate the interpretations among sites (general consistency check). For example, does the descriptive conceptual model that explains the existence of a diffusion profile at one site also explain the absence of such a profile at another site.
- To fit model calculations to measured tracer distributions and thereby constrain the large-scale diffusion coefficients or diffusion times. If independent evidence exists on the latter, diffusion coefficients can be obtained by fitting predictive model calculations to observed data. These large-scale values can then be compared with laboratory measurements on small samples and thus contribute to the issue of upscaling to PA-relevant scales.
- To judge the relevance of observed geological discontinuities, such as faults, for flow and transport over long periods of time in the past.

Hydraulic and transport properties of argillaceous formations can be addressed by different lines of evidence, such as hydrogeological investigations (e.g. hydraulic packer tests and long-term monitoring) or geological arguments (e.g. the presence/absence of vein mineralisations and wall-rock alterations that would indicate fluid flow in the past). The quantitative evaluation of tracer distributions may add another independent line of evidence.

Pre-requisites for a quantitative evaluation of tracer profiles

The investigation and quantitative interpretation of tracer profiles requires three basic types of input data ("pillars"):

Pillar 1: Data on the spatial distribution of conservative tracers (profiles of anion and noble gas concentrations and isotopic compositions of water across the argillaceous formation).

Pillar 2: Knowledge of relevant formation properties, such as:

- System geometry.
- Porosities.
- Diffusion coefficients.
- Heterogeneity and anisotropy.
- Location of faults and joints.

Pillar 3: Palaeo-hydrogeological understanding to constrain initial and boundary conditions for diffusion, notably:

- "Early" site-specific geochemical and hydrogeological evolution.
- Dating the onset of exchange with bounding upper and lower aquifers.
- Evolution of boundaries with time.

Current status

Formations and sites considered in the project include the Callovo-Oxfordian at Bure, the Toarcian-Domerian at Tournemire, the Couche silteuse at Marcoule (all France), Opalinus Clay at Benken and at Mont Terri (Switzerland), London Clay at Bradwell (UK), Boom Clay at Mol (Belgium) and Canadian Quaternary tills. The availability of data varies among sites and formations. If available, the following tracers are considered: Cl, δ^{37}Cl, Br, I, δ^{18}O, δ^{2}H and He. At the present stage, no final results are available yet. Activities to date have been as follows:

- Data needed for an improved understanding of spatial tracer profiles have been compiled. The compilation was based on published literature, on openly accessible reports as well as on unpublished information provided by the organisations that are responsible for the characterisation of the various sites. This process, including the direct interaction with the data producers, has been running well and is close to completion.
- A stage of data processing is needed in order to derive an internally consistent data set suited for numerical simulation. Examples include the definition of solute-specific porosities to calculate solute concentrations in pore water, or a consistent consideration of anisotropy of diffusion coefficients.
- To date, various numerical modelling tools have been used for the quantitative evaluation of tracer profiles. The processes and the geometric complexity considered vary among codes. However, until now, no single code has satisfied all the requirements of CLAYTRAC, namely:
  - consideration of internal heterogeneity (sedimentary layers with different properties, faults);
  - consideration of a material anisotropy (bedding);

- consideration of variable boundary conditions over geological time (e.g. dependence of the isotopic composition of meteoric water as a function of climate, or changing Cl contents in bounding aquifers due to erosion, marine trans- or regression);
- consideration of *in situ* production of He by radioactive decay of U and Th;
- graphic interface for the visualisation of modelling results;
- routine to fit model calculations to measured data;
- 1-D and 2-D capabilities.

In the framework of CLAYTRAC, the finite difference, 3-D transport code FLOTRAN (Lichtner 2004) was selected and adapted in order to satisfy all the requirements listed above. Adaptations included mainly the introduction of anisotropic transport properties and a source term to account for *in situ* production of He. A graphic interface was linked to the code for the visualisation of model results (pictures and movies), and a least-square fit routine has been implemented. While only conservative tracers are considered in the framework of CLAYTRAC, FLOTRAN also has the capability to model quantitatively fully coupled, multidimensional reactive transport (including sorption and reaction kinetics).

Example

The Mont Terri Rock Laboratory (Jura Mountains, NW Switzerland) penetrates Opalinus Clay, an indurated argillaceous formation, which is embedded between two limestone aquifers. In an extensive study targeted at the characterisation of the pore waters, Pearson *et al.* (2003) documented the spatial distributions of Cl, δ^{37}Cl, Br, I, δ^{18}O, δ^{2}H, He and ^{40}Ar/^{36}Ar in pore water across the formation (Pillar 1 above), relevant formation properties such as porosity and solute-specific effective diffusion coefficients and the location of major faults (Pillar 2), as well as the chemical and isotopic compositions of the ground waters in the aquifers and information on palaeo-hydrogeology (Pillar 3).

Profiles of Cl and He in pore water are shown in Figure 1. The common aspect of both profiles is that tracer contents are high in the Opalinus Clay and decrease towards the bounding aquifers, where the values are close to zero. The He profile is near-symmetric, with a maximum value in the centre of the formation. In contrast, the maximum Cl content (about 0.75 x sea-water composition) is found close to the lower boundary, towards which the concentration drops rapidly over less than 50 m. The decrease of Cl contents towards the upper boundary is more gradual. Both profiles are reasonably smooth and completely unaffected by the presence of a major fault with an extension in the order of ≥100 m that penetrates the profile.

The erosion history of the Mont Terri anticline (Figure 2) implies that the limestone aquifer overlying Opalinus Clay became exposed on the surface some 2.5 Ma b.p. It is likely that, at this stage, a ground-water circulation started and flushed the aquifer with fresh water. The lowermost Jurassic aquifer underlying Opalinus Clay was exhumed only ca. 0.35 Ma b.p. Preliminary calculations considering the different times at which the flushing of the aquifers was initiated are capable of explaining the observed asymmetry of the Cl profile. Assuming diffusion to be the only transport process and using an effective diffusion coefficient for Cl derived from laboratory experiments yields build-up times for the observed Cl distribution consistent with the erosion history as shown in Figure 2.

Figure 1. **Tracer distributions in pore water of Opalinus Clay at Mont Terri, Switzerland. Data from Pearson *et al.* (2003).**

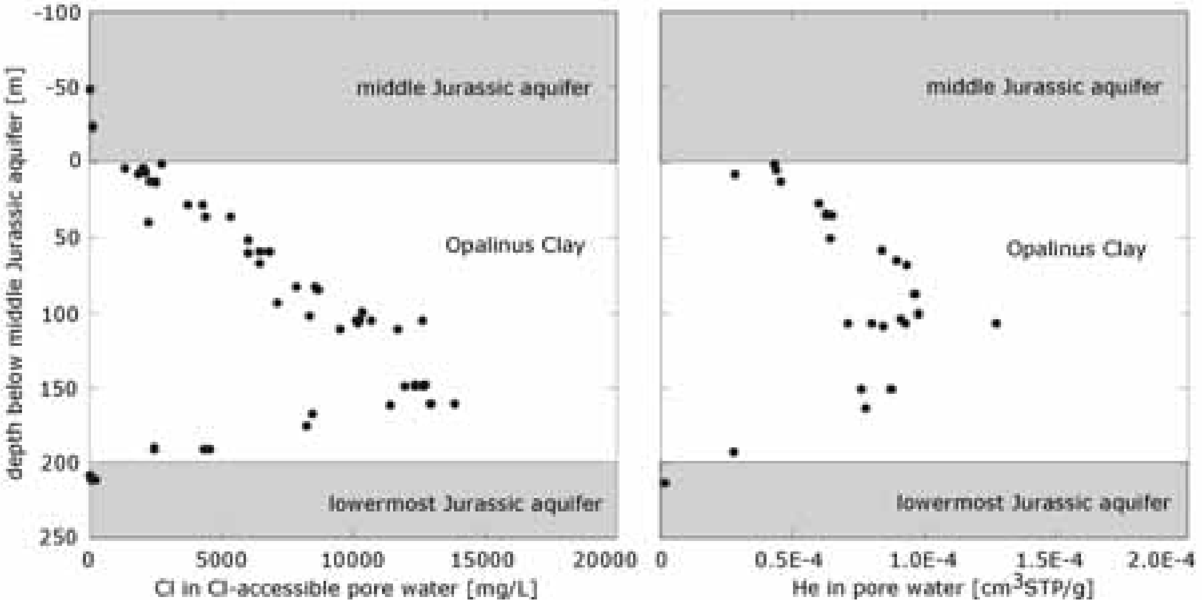
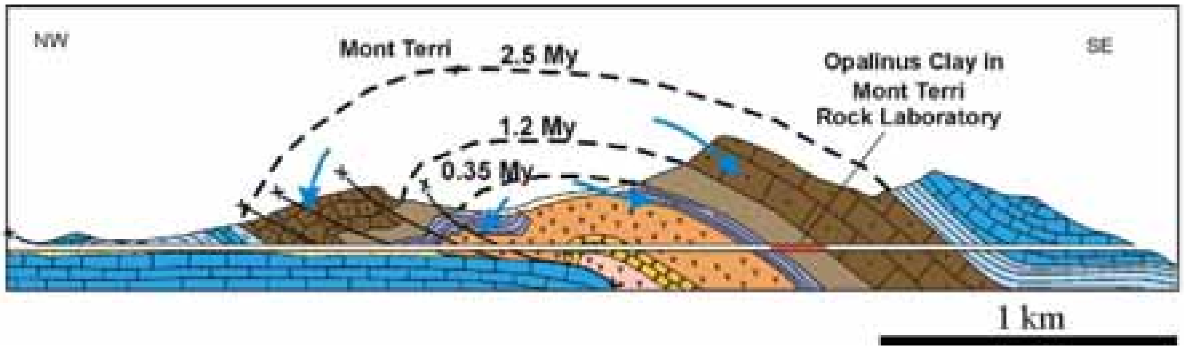


Figure 2. **Erosion of the Mont Terri anticline, from Pearson *et al.* (2003).**



The consistency between observation and model prediction is a necessary but not sufficient argument supporting the assumption of a diffusion-dominated system and the validity of laboratory-derived diffusion coefficients for in-situ conditions. Further confidence in this conceptual model can be gained by testing it against other data, such as the distribution of other tracers. Thus, the same model needs to explain the asymmetry of the Cl profile and the symmetry of the He profile. For the latter, *in situ* production has to be considered as an additional process, and a higher diffusion coefficient and a larger accessible porosity need to be taken into account. Calculations testing the internal consistency of the conceptual model and data set are under way.

Link to the objectives of the AMIGO project

The evaluation of natural tracers requires a co-ordinated, integrative effort including:

- the design and execution of adequate field sampling (using purpose-designed procedures and devices);
- the measurement of relevant parameters in the laboratory (often using non-standard techniques);
- the characterisation of the palaeo-hydrogeological evolution of each site by independent methods;
- numerical modelling by which the knowledge on spatial tracer distributions, formation properties and boundary conditions changing over time is integrated.

In the ideal case, the approach contributes to:

- demonstrate, on an international basis, the utility of the technique in supporting both the development of descriptive conceptual models in the safety case and building confidence in predictive estimates of geosphere barrier longevity and performance;
- explore issues related to mechanisms of mass transport and to upscaling of parameters to time and space scales relevant to repository safety;
- demonstrate the resilience of the formation to external perturbations (i.e. long-term maintenance of diffusion dominated mass transport regime);
- communicate concepts of geosphere stability and longevity that are less evident to wider audiences when considering safety assessment calculations alone.

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USE OF GEOSCIENTIFIC ARGUMENTS IN THE NIREX PHASED GEOLOGICAL REPOSITORY CONCEPT: ILLUSTRATIVE DESK STUDY

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Generally, a performance assessment (PA) will include a range of quantitative performance indicators, together with alternative lines of reasoning and qualitative considerations, to build understanding in the overall repository performance and hence determine whether it satisfies the relevant safety requirements [1]. Although the quantitative evaluation of performance continues to be important, recently there has been an increasing recognition that qualitative arguments also have an important role to play in establishing and communicating confidence in the safety of repository systems. There is also a role in many PAs for semi-quantitative arguments, for example applying physical and chemical understanding of the system to build "insight" models of repository system behaviour.

A desk study recently undertaken by Nirex used data, collected from now-ceased investigations of the Sellafield site (west Cumbria, UK) undertaken in the 1990s, to consider the implications of locating the Nirex Phased Geological Repository Concept[1] (PGRC) in deep rock formations present at the west Cumbrian coast that contain brines in a slow-moving groundwater flow system. Work undertaken brought together geochemical data and interpretation [1], addressing some questions that were posed during active Sellafield investigations concerning the distribution, composition, origin and age of the brine. The desk study also considered geochemical evidence that has a bearing on understanding the hydrodynamic stability of the brine, noting that it has been investigated in a zone where there are quite sharp changes in physical and chemical groundwater conditions over rather short distances; the simplified hypothesis that this brine is "very old and virtually immobile" is considered. Other important parts of the scientific framework that provide complementary knowledge and insights were utilised for this desk study; physical hydrogeology and numerical modelling, basinal geology, structure and rock properties, and mineralogy were integrated with geochemistry to develop an understanding of the behaviour of the groundwater system in the study region in terms of its evolution to present day, and its potential future behaviour.

The following conclusions of the desk study are reported in references [2, 3, 4].

- There is a coherent volume of brine groundwater at depth under the coast of west Cumbria that almost certainly is continuous westwards into the East Irish Sea Basin (though there are no borehole data in the immediate offshore area).

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[1] This concept considers the UK's intermediate level and long-lived low-level radioactive wastes. In the reference conceptual design, the repository is envisaged as being constructed at a depth of c.650 m in hard fractured rock overlain by a sedimentary succession. The host rock provides low groundwater flow through the repository; the geosphere provides a long groundwater return time. Assessments of the groundwater, gas and human intrusion pathways are undertaken; the groundwater pathway discharges to land.

- Integrated interpretation of various strands of geochemical/isotopic data strongly indicates that the water in the brine is at least 1.6 million years old, i.e. prior to the Quaternary period. Palaeohydrogeological considerations suggest that it most probably originated as meteoric infiltration to groundwater during the Tertiary period (between 1.6 and 65 million years ago). Being that old, there can be little doubt that the present brine is now a complex mixture of waters with no identifiable discrete origin.
- Ancient water became salinised to a brine because it dissolved halite principally from the Triassic Mercia Mudstone Group which is known to have thick salt beds in the centre of the geological basin.
- Preservation of fracture-filling secondary anhydrite suggests that highly saline groundwater conditions have persisted west of the present position of the brine-saline water transition and mixing zone (movement of this zone to the east is not precluded).

Semi-quantitative and qualitative comparison between hydrodynamic and geochemical estimates of water ages are reported in [4]. The main assumptions and simplifications in each case that affect the degree of comparability are described in that report, and the consistencies and inconsistencies are discussed and reconciled as far as possible. Geochemical ages for time since recharge of the water in the brine are upwards of 1.6 million years. A probable maximum age of 10 million years is inferred from an assumption about how groundwater history might be coupled to geological history.

Taking into account the uncertainties in model parameters, geometry and the steady state assumption in the hydrodynamic model, and the semi-quantitative nature of the geochemical ages, an average age range of 2 to 10 million years for water in brine at the west Cumbrian coast is the most reasonable conclusion. The hydrodynamic model and the geochemical data are both consistent with that estimate.

This degree of consistency between geochemical ages and brine travel times gives more credibility to the hydrodynamic model used to estimate return times from points at various depths under the coast to the surface. The modelled travel times from various depths under the coast to discharge at the present day seabed are 10^5 to 10^6 years, depending on the value used for transverse dispersivity and many other factors

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PAST GEOLOGIC, CLIMATIC AND GEOMORPHOLOGIC FORCING INFLUENCE ON PRESENT-DAY HYDRODYNAMICS, A KEY TO UNDERSTANDING FUTURE EVOLUTION: EXAMPLE OF THE PARIS BASIN, FRANCE

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1. Introduction

The evaluation of the influence of future climatic and morphologic changes on the hydrogeology of sedimentary basins, to support hydrodynamic modelling for a nuclear waste disposal safety assessment, requires:

- an extensive data set capable of reproducing hydrodynamic parameter heterogeneity;
- identification and quantification of the mechanisms likely to affect the hydrodynamics; and
- appropriate initial hydrodynamic conditions.

To this end, the well known Paris basin can be considered a "*textbook case*" as many scientists from different fields have studied it over the past decades. A large amount of diverse data is therefore available.

The reconstruction of past forcing, such as changes in geology, climate and morphology, and its contribution to present-day hydrodynamics, is a scientific challenge. One crucial question is: *How far back in time must we go to build a coherent hydrodynamic model?* We propose and discuss some options in this presentation.

2. Approach

To reproduce hydrodynamic parameter heterogeneity at the basin scale, the potential applications include [1]:

- continuous geostatistical models;
- discontinuous facies models such as the Boolean, Indicator or Gaussian-Threshold models and the Markov chain model; and
- inverse hydrodynamic models.

In general, the paucity of hydrodynamic data available at this scale seriously limits the predictive power of any approach, especially for aquitards and deep aquifers. To alleviate this lack of hydrodynamic data, we used a genetic-based modelling approach which integrated geological data (from a database of more than 1 100 petroleum litho-stratigraphic well logs) and reproduced hydro-thermo-mechanical processes over 248 My of history for the Paris sedimentary basin [2]. To assess the accuracy of the simulation results, diagenetic constraints had to be respected [3,4] and upscaling of the available hydrodynamic data had to be done before validation.

From the results obtained, hydrodynamic parameter implications include the following:

- satisfactory equivalent and regional-scale permeabilities are calculated by the code;
- a better knowledge of lithology increases the quality of calculated permeabilities;
- integration of petrophysical laws adapted to the type of sediments, such as the Lucia Law for carbonates [5] and the Kozeny-Carman equation for detritic sediments [6], improves estimation of the heterogeneous distribution of permeabilities; and
- the data at all scales, and scale effects, are important.

Thus, a 3-D hydrodynamic model of the entire Paris basin extended towards the North (London basin) and the West (Germany) was developed for predicting the shorter time scale past evolution or the future evolution.

Prescribing accurate initial hydrodynamic conditions is one of the trickiest parts, as nowadays water level records in many aquifers are strongly influenced by human exploitation for water, oil, gas and heat. Only the Albian aquifer has water level records reaching back before the start of its exploitation [7]. The few available data in aquitards show low overpressures (e.g. in the Callovo-Oxfordian, 0.2-0.5 MPa, equivalent to 20-50 m of excess head) and their origin is still under debate.

In such a context, several likely mechanisms can be invoked:

- gravity-driven flow; [8]
- changes in hydrodynamic conditions under tectonic, morphologic or climatic forcing;[8,9]
- compaction disequilibrium; [9,10]
- water genesis by hydrocarbon transformation; [8]
- clay dehydratation; [9,11]
- visco-plastic behaviour of clay; [12,13] and
- osmosis. [8,14]

In the Paris basin context, compaction disequilibrium can be ruled out as overpressures generated during geological history are weak and rapidly dissipated [14] (100 ky to 1 My after sediment deposition had stopped). The rapid dissipation of overpressure is also an argument for eliminating diagenetic processes. Understanding of visco-plastic and osmosis [15] processes is growing but still incomplete. In this study, we focus our attention on the past climatologic and geomorphologic forcing which may have induced transient fluid flow, of which low-permeability layers may have kept the memory. Another fact which encourages us in this approach is that water tracers (such as the rare gases ^{18}O and ^{2}H) in deep aquifers have kept the memory of past recharge under lower temperatures (~12°C less than present-day recharge temperatures) likely to have occurred during the Last Glacial Maximum (~21 ky BP) [7,16,17,18]. However, only a few studies [19,20,21] deal with the effect of changes in the amount of past recharge. From these studies, the presence and melting of permafrost, which reduces or even prevents recharge during glacial periods, seems to be the mechanism most likely to produce transient fluid flow that has still not dissipated at the present time in low-permeability layers.

To test the impact of past climate and morphology on present day hydrodynamics, we reconstructed scenarios of their past evolution. The fluctuation in ^{18}O in foraminiferan shells extracted from deep ocean cores, such as ODP.659 [22], is an indicator of the global climate evolution over the last 5 My. The Plio-Pleistocene period is characterized by a global cooling trend that led up to the Quaternary ice ages. Between 2.6 and 0.9 My, the climatic record is dominated by 41-ky oscillations. There is a major climate shift near 0.9 My after which the length and amplitude of the cycle increased to 100 ky. During the last 5 My, the geomorphologic evolution of the Paris basin is linked to tectonic movements in relation with the Alpine uplift, and to climate and eustatic variations of the Plio-Pleistocene. Starting from a smooth topographic surface where large braided systems occurred, the morphologic evolution has resulted in a slow uplift of the basin [23,24] and river-valley incision which began around 1 My ago [25]. According to the past evolution and to the dissipation time of perturbations, the 5 My duration allows us to disregard older potential transient phenomena and yet ensures we include any effect induced by the 41-ky and 100-ky climate oscillations.

To complete our approach, quantitative palaeo-climate and morphologic scenarios have been built up over the last 5 My [26,27]. The global climate evolution described by the ODP curve has been used to identify a set of main stages of stable climatic conditions. In order to quantify the climate forcing and its spatial distribution, palaeo-climate modelling experiments were undertaken at key chosen periods: present day (CTRL), Last Glacial Maximum (LGM: 21 ky BP), and Middle Pliocene (MPL: 2.6 to 2.4 My BP). Model responses were compared to an updated pollen data base. This pollen data base was also used to interpolate climatologic variables such as rainfall and potential evapotranspiration over time at each stage. Then these variables were converted as an input for a groundwater model (NEWSAM [28]) using a distributed hydrological model (MODSUR[28]) to compute the water budget. A geomorphologic scenario was deduced from digital elevation model analysis, which allows us to quantify river-valley incision and alpine uplift. Mean sea-level values for each climatic stage are deduced from the Greenlee and Moore curve [29].

3. Results

The 3D hydrogeological model was used to reproduce the transient response to changes in hydrodynamic boundary conditions during Plio-Pleistocene times [26]. The geometrical and hydrodynamic representations of the basin are based on the basin model simulations [2], with a reduced extension: Paris and London basins *sensus stricto* including the Channel sea (covering a total surface of 250 000 km^2). To determine a set of consistent initial conditions at 5 My, a reference steady-state simulation was made to provide the hydraulic head distribution, from which the time evolution of the system was calculated. The hydrodynamic state of the system was recorded every time step (1 000 y). The model generates the distribution of hydraulic heads through the Plio-Pleistocene history of the entire Paris basin (20 layers). The calculated head distribution given by the transient simulation at the present time was compared with the results of a steady-state calculation for the present conditions, to evaluate the possible presence of transient pressure remnants due to past changes in the boundary conditions. First, a sensitivity analysis of model parameters on the differences between the two head distributions was carried out. Second, a sensitivity analysis of each individual mechanism was made over the last 100-ky cycle, with a shorter time step (100 y) and special attention to the permafrost representation.

Modification of recharge is the most likely mechanism which seems to have an impact on hydraulic head differences, notably the absence of recharge during the permafrost period. This is emphasise by the water balance analysis of low permeable layers during the last cycle, which reveal the modification of leakage flux direction. Topographic modifications have a low effect on hydraulic head changes, and sea level fluctuations have a transient effect localized along the sea coast. Results show a rapid dissipation of perturbation in aquifers while aquitards keep longer memory of their effect, i.e. in the range of several 10 ky depending on the diffusivity of the considered formation, if this diffusivity is lower than 10^{-6} to 10^{-7} $m^2.s^{-1}$. An inter-glacial state over the last climate cycle, lasting less than 10 ky, is also a predominant factor in maintaining a transient regime. Our results show that the Paris basin is definitely not at equilibrium with present-day climate and topographic conditions. Its present transient hydrodynamics are a consequence of past glacial and inter-glacial oscillations. A cumulative effect of past perturbations in a formation is only possible if the return period of the perturbation is short or the characteristic dissipation time of the formation is long. In such conditions, the system memory can extend over 1 My.

4. Conclusions

To conclude, present-day Paris basin hydrodynamics are influenced by past climatic and morphologic forcing. The system is not in a steady-state regime, even if conditions occurring before any aquifer exploitation are considered. Initial conditions for modelling the future evolution of the basin under any new forcing cannot be taken as steady-state, as is usually done.

We have shown so far that:

- 248 My of geological processes have to be taken into account to reproduce an accurate geometry and hydrodynamic parameter heterogeneity at the basin scale,
- the 5 My duration allows us to disregard older transient phenomena which may had occurred, and
- a shorter period of 1 My can now be used to better describe processes such as permafrost, which seems to have the largest influence.

Accurate representation and understanding of permafrost could also be used in prospective hydrodynamic modelling under future glacial conditions.

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SPATIAL EXTENSION AND PARAMETER INTEGRATION INTO THE SAFETY CASE – EXAMPLES FROM THE HUNGARIAN LLW/ILW AND HLW DISPOSAL PROJECTS

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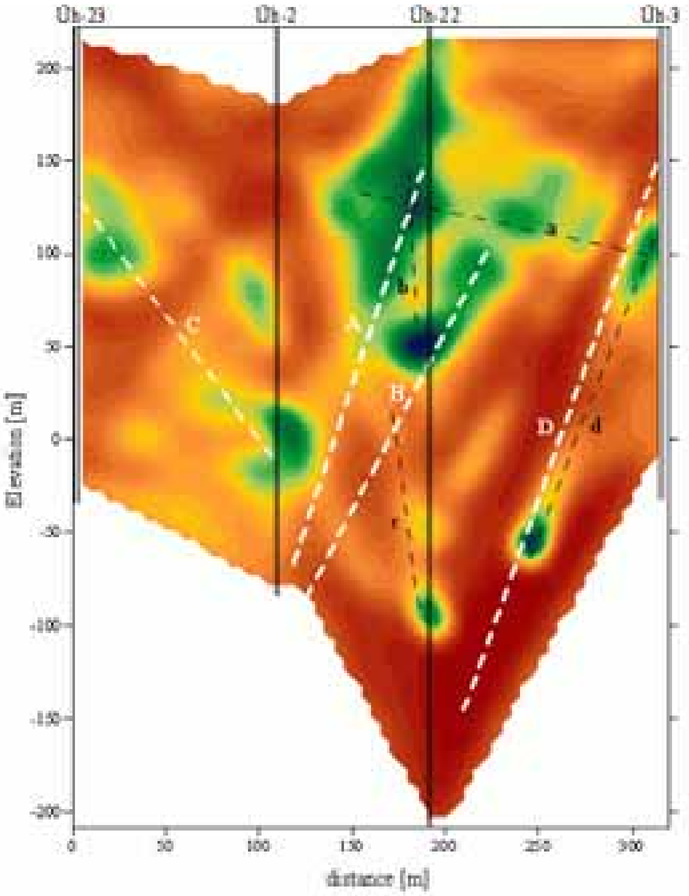
Exploration of potential sites for radioactive waste disposal of waste types LLW, ILW and HLW is underway worldwide. Nuclear disasters of the last decades and their spatial effects and temporal decay show that the long term safety of radioactive waste disposal systems, including recognition and modelling of future events, is of the highest importance. A key outcome of these site investigations is the generation of information required by Safety Cases, notably the identification of how future events might affect safety. Models developed for studies of safety must describe complex systems over long time frames and thus must deal with measured and calculated parameters and their associated uncertainties. However, there are some basic problems, especially in the first phase of the research, when the limited available information must be extended spatially and the uncertainties might not be well understood. This presentation will discuss two examples in connection with research on potential host rocks for Hungarian LLW/ILW and HLW disposal: the feasibility of parameter spatial extension and estimation of the uncertainty of permeability.

The first example pertains to geological research on the Mórágy Granite Formation (MGF), a potential host rock for Hungarian LLW/ILW disposal in Bátaapáti, and is concerned with the interdependent use of geological and geophysical information. During this project, boreholes were drilled and cores were analysed with general and special geological and geophysical methods. Indirect connections between physical parameters provided by geophysical measurements and geological characterisation of the different parts of MGF supported the estimation of spatial variability of the granite body. However, this is not unique correspondence of geological structures. Depending on the resolution of the applied geophysical method, a given space domain is characterised by an average value of the measured parameter. Seismic tomography was one of the best methods for parameter extension (Figure 1). Its applicability, advantages, disadvantages and further investigations will be discussed in this presentation.

The second example deals with geological research on the Boda Claystone Formation (BCF), a potential rock body for HLW disposal in Hungary and describes a new laboratory method for gas and water permeability measurement. The well-conditioned cores originated from the so called Alpha-1 exploratory tunnel – a deep level Underground Research Laboratory (URL) in the BCF which has been already backfilled. These cores provide an opportunity to investigate different laboratory procedures to measure hydrodynamic parameters such as porosity, pore size distribution, and gas and water permeability. This is challenging task because previous results have indicated that the porosity of the BCF is between 0.5 to 3.0%, gas permeability ranges from 10^{-18} to 10^{-20} m^2, and water permeability values, measured in same cores are about 2 orders less in magnitude than gas permeability. Using traditional techniques based on Darcy’s equation, measurement of permeability, especially water permeability, can only be carried out on a long time scale. Results from these measurements cannot be characterised statistically because of the small sample size (only 1 to 3 measurements in the same core).

Moreover, there is a general problem with respect to laboratory measurements in that formation conditions (temperature (T), pressure (p) and water composition) cannot be established in most cases. For permeability measurements of BCF cores, a special permeameter was developed which can be applied for either gas or water permeability measurements under “quasi real” formation conditions, i.e. a temperature up to 35°C (95 °F) and a pressure of 60 to 80 bar (870-1160 psi). The working principle of the permeameter is based on the theory of pressure pulse decay. Using this tool, gas and water permeability of the BCF was measured over a few minutes and 1 to 3 hours, respectively. With revision of our own specially-designed computer program, interpretation was carried out which can handle the parameter calculation, Table 1 shows some results which include statistical uncertainties of parameters. These results show good agreement with previous data and thus may be integrated into the Safety Case with higher precision.

Figure 1. **An example for parameter extension by seismic tomography at Bátaapáti site, Hungary.**



Üh-23, 2, 22, 3 are boreholes

A, B, C, D are the indications of main structural inhomogenities

a, b, c, d are the additional indications from absorption tomography

colour scale: values of absorption from blue (max.) to red (min.) with dynamic range of 40 dB

Table 1. Hydrodynamical parameters of the BAF-2/2 sample at different pressure and temperature.

	Porosity* [%]	**T [°C]**	**$p_{2\text{-mean}}$ [bar]**	**p_h-$p_{2\text{-mean}}$ [bar]**	**$k_{g\text{-}2\ med}$ [m^2]**	**$k_{g\text{-}2\ mean}$ [m^2]**	**σ [+/-]**
gas permeability	2.12	34.47 ± 0.07	79.95	21.0 ± 0.3	$1.33\cdot10^{-19}$	$1.33\cdot10^{-19}$	$3.1\cdot10^{-21}$
		34.49 ± 0.06	79.23	21.6 ± 0.2	$1.34\cdot10^{-19}$	$1.34\cdot10^{-19}$	$2.1\cdot10^{-21}$
		34.30 ± 0.06	69.02	21.4 ± 0.3	$1.26\cdot10^{-19}$	$1.26\cdot10^{-19}$	$3.0\cdot10^{-21}$
		34.83 ± 0.06	68.38	21.0 ± 0.3	$1.28\cdot10^{-19}$	$1.29\cdot10^{-19}$	$2.9\cdot10^{-21}$
		34.72 ± 0.07	57.91	20.9 ± 0.2	$1.24\cdot10^{-19}$	$1.24\cdot10^{-19}$	$3.0\cdot10^{-21}$
		34.61 ± 0.03	48.61	21.1 ± 0.2	$1.20\cdot10^{-19}$	$1.20\cdot10^{-19}$	$2.5\cdot10^{-21}$
		35.00 ± 0.03	38.33	21.6 ± 0.2	$1.17\cdot10^{-19}$	$1.17\cdot10^{-19}$	$3.2\cdot10^{-21}$
					$k_{w\text{-}2\ med}$ [m^2]	**$k_{w\text{-}2\ mean}$ [m^2]**	**σ [+/-]**
water permeability	2.12	35.00 ± 0.09	67.69	22.3 ± 0.7	$1.42\cdot10^{-20}$	$1.41\cdot10^{-20}$	$1.6\cdot10^{-21}$

* calculated porosity at atmospheric conditions (27.4 °C, 1.01 bar)

$p_{2\text{-mean}}$ is the average value of the pore pressure

p_h is the hydrostatical pressure

$k_{g\text{-}2\ med}$ is the median of permeabilities

$k_{g\text{-}2\ mean}$ is the average value of permeabilities

σ is the standard deviation related to average values

COMPLEX BRANCHING STRUCTURES IN CRYSTALLINE ROCK: TREATMENT OF UNCERTAINTY IN SAFETY ASSESSMENT

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For a deep radioactive-waste repository hosted in granitic bedrock, highly fractured fault zones (whether ancient or modern) are likely to serve as the dominant conduits for groundwater flow affecting geochemical conditions at repository depths and radionuclide retention in the event of engineered-barrier failure. Fault zones also affect geomechanical stability, as the most likely loci of displacements in the event of future tectonism. Determining adjacency to fault zones, and assessing their impact on repository components, are thus important components of a safety case for a repository in granitic rock.

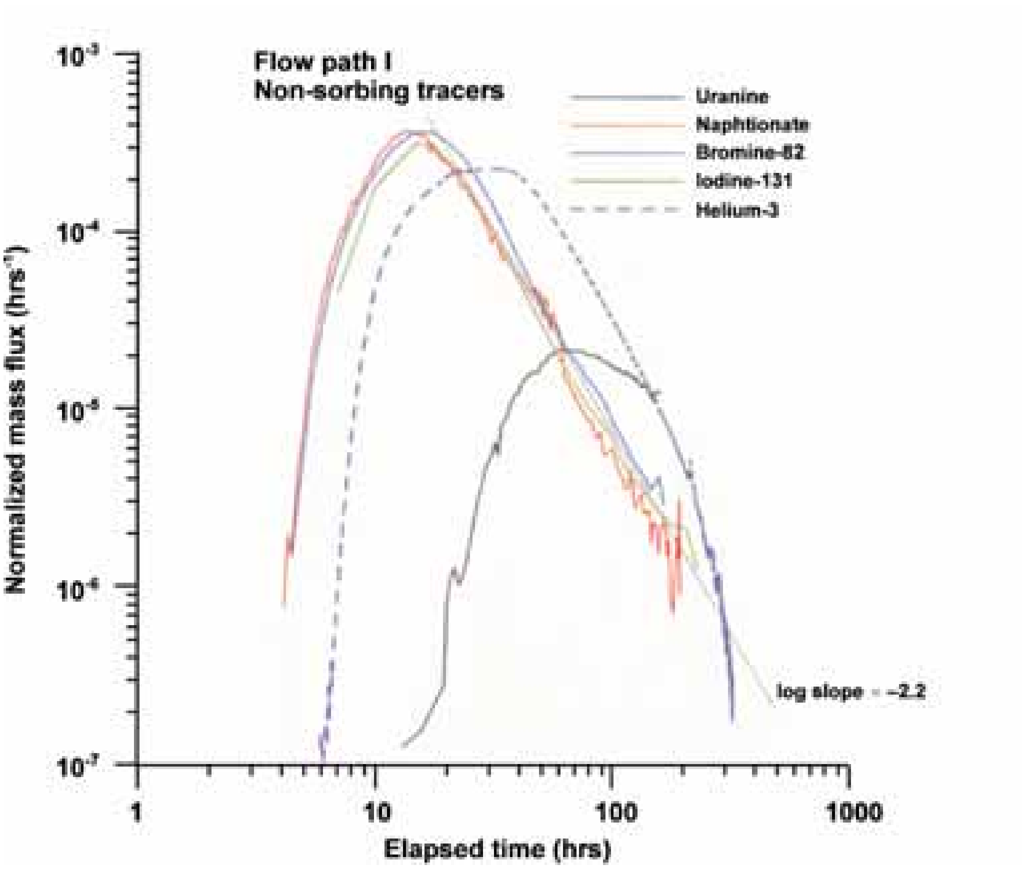
Field studies of fault zones, as recently surveyed by Kim *et al.* (2004), have led to a view of fault zones as complex structures with characteristic, hierarchical geometric properties that are observed over scales of centimeters to hundreds of kilometers. Key aspects of fault-zone geometry for repository safety assessment include (1) the tendency of faults to be linked en échelon, (2) the tendency of faults to have "damage zones" of increased fracturing adjacent to the main fault surfaces, and (3) the tendency for the fractures within the "damage zones" to be organised as a hierarchical system of subsidiary faults and joints.

This paper presents recent results on the effects of hierarchical fault-zone geometry on radionuclide transport, based on detailed outcrop studies from two granitic sites in Sweden (Geier, 2004). Hierarchical fault-zone geometry has been observed in a wide range of rock types, but the present analysis is limited to the case of granitic, crystalline rock. Results of numerical modelling show that the observed, hierarchical pattern of branches yields fractal-type scaling of the pore volume that solute can access by diffusive mass transfer, with increasing distance from the main fault segments.

Effects of hierarchical branching structures can include tailing of solute breakthrough curves similar to that observed in underground tracer experiments. For example, analysis of branching characteristics on an en échelon structure exposed on outcrop at the Äspö site in Sweden, as detailed by Geier (2004), yields a predicted late-time negative log slope of 2.2 for tracer breakthrough (if the fractal dimension of the branching is assumed to persist over scales 1-2 orders of magnitude smaller than the 1 cm resolution of the mapping). This is very close to what has been observed in tracer tests on a similar-oriented structure at depth (Figure 1).

Branching structures are furthermore shown to yield additional retention capacity beyond simpler models of fault zones. The additional access to the matrix provided by the stagnant branches can enhance the retardation due to matrix diffusion by up to a factor of two, based on network simulations for head gradients and time scales that are representative of post-closure repository safety assessment. This marginal increase is not likely to be significant in terms of safety assessment.

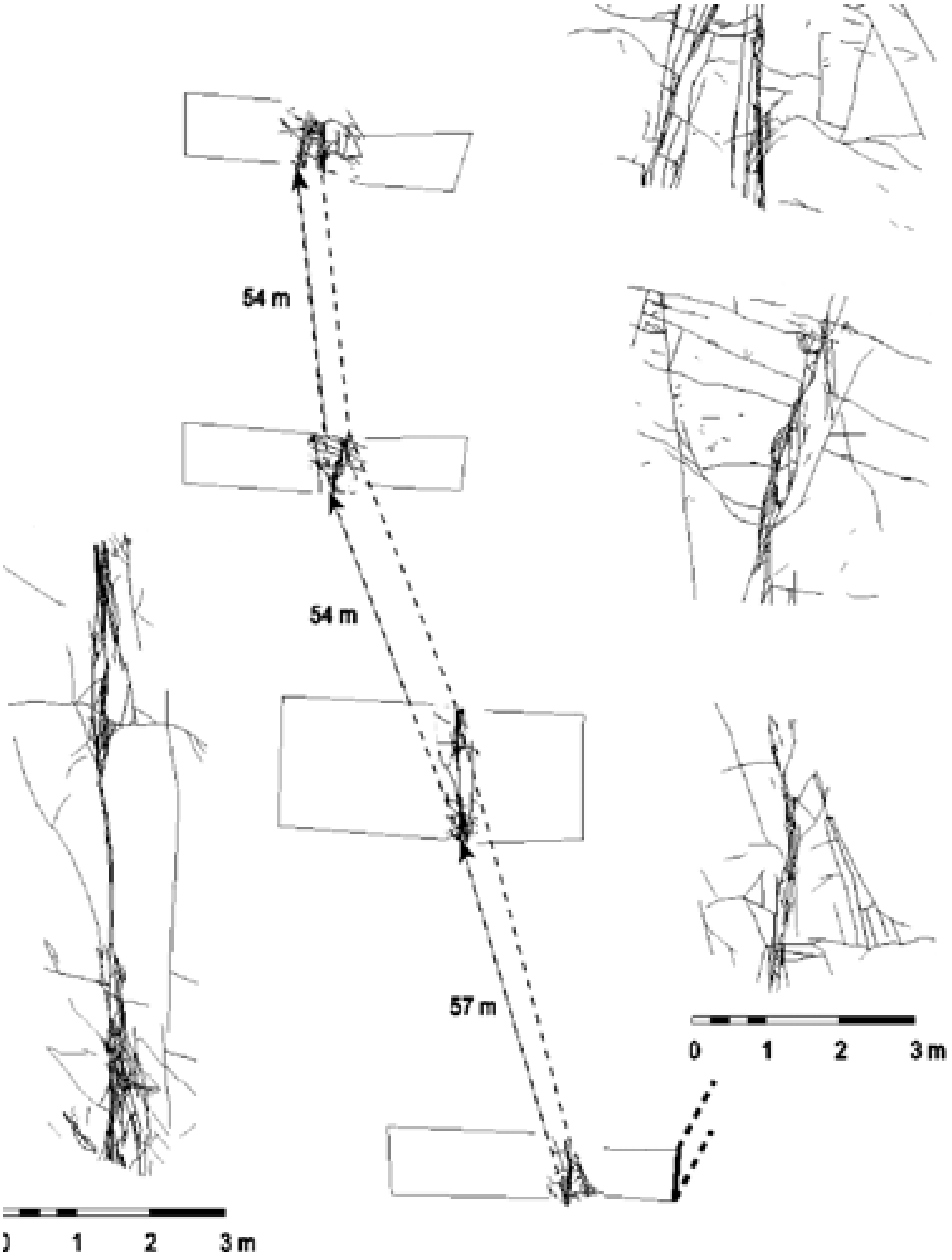
Figure 1. **Normalised breakthrough curves for conservative tracers in Flow Path I during the TRUE Block Scale experiments in the Äspö Hard Rock Laboratory, showing graphical estimate of late-time log slope (modified from Winberg *et al.* 2002).**



However, the role of branch fractures can be important to recognise in extrapolating from short-term tracer experiments to time scales of models used in safety assessment. For example, if retardation due to diffusion into stagnant branch fractures during a tracer experiment is incorrectly attributed to matrix diffusion, but those branch fractures are included in estimates of the flow wetted surface through which diffusion into the matrix can occur, less conservative estimates of retention parameters may result. The time-dependency of immobile volumes accessible to solute in a branching network will also affect comparisons between tracer experiments conducted on time scales of days to weeks, vs. natural tracers which percolate through the rock on time scales of many years.

Hierarchical fault-zone geometry may have practical significance for repository safety cases in other respects. The hierarchical geometry affects the concept of "respect distance," i.e. the distance at which radioactive waste can presumably be emplaced with minimal concern for the fault zones. Smaller faults are likely to be connected to larger faults as part of a hierarchical system, and thus may be linked both geomechanically and hydrogeologically to the larger faults. Examples are given of secondary faults in branching systems which extend beyond respect distances that have been used in recent safety assessment exercises, including examples from the literature as well as an apparent splay fault which was characterised in detail at the Ekolsund, Sweden study site (Figure 2).

Figure 2. **Fracture maps of four vertical exposures along a single interpreted, N-striking fracture zone at the Ekolsund site in south-central Sweden. Overview in centre of plot is isometric view of the four road-cut exposures, viewed in the direction N15E and 20 degrees downward from horizontal. The median surface of the zone, as indicated by the dashed lines connecting between panels, is itself interpreted as a splay of a larger, NE-striking fracture zone (indicated by thick blue lines) which crosses the southernmost exposure just east of this zone, based on topographic lineaments and geophysical profiles.**



In field characterisation, it may furthermore be difficult to ascertain whether a small fracture that is detected near a waste deposition hole is simply an isolated fracture, or part of a hierarchical fault system. Conventional, Poissonian models of discrete-fracture networks, in which fractures are treated as essentially independent entities, may be optimistic rather than conservative when used to assess strategies for deposition-hole siting within a repository. A given fracture in a hierarchical model is more likely to connect to a large-scale structure than a given fracture in a Poissonian model, and thus may be more susceptible to disturbances along larger-scale structures and/or form part of a path with less favourable radionuclide retention properties. It is therefore suggested that an analysis of possible hierarchical fault-zone geometry should be performed as part of fracture-network characterisation, to determine if hierarchical models would provide more realistic tests of waste deposition strategies than conventional, Poissonian models.

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ASSESSMENT OF UNCERTAINTY AND CONFIDENCE IN SITE DESCRIPTIVE MODELS – EXPERIENCE FROM THE ONGOING SITE INVESTIGATION PROGRAMME IN SWEDEN

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Abstract

SKB, the Swedish Nuclear Fuel and Waste Management Co, is currently pursuing surface based site investigations, for a deep spent fuel repository of the KBS-3 type, in the crystalline basement rock at the Forsmark area in the municipality of Östhammar and at the Simpevarp and Laxemar subareas in the municipality of Oskarshamn. The investigations are conducted in campaigns, data freezes, and after each data freeze Site Descriptive Models (SDM) are prepared. A Site Descriptive Model is a synthesis of geology, rock mechanics, thermal properties, hydrogeology, hydrogeochemistry and a surface system description. Eventually, this synthesis will form part of the Safety Case in the license application and is also used for preparing repository layouts and as input to the Safety Assessment.

So far, two versions of SDM (versions 1.1 and 1.2) have been developed for both the Forsmark area and the Simpevarp subarea. Version 1.1 for both the Forsmark area and the Simpevarp subarea was completed during 2004 and version 1.2 approximately one year later, in April 2005 for the Simpevarp subarea and in June 2005 for the Forsmark area. Version 1.2 of the SDM conclude the Initial Site Investigation phase (ISI) and form the basis for preliminary repository lay-outs, as well as for preliminary safety evaluations of the sites. In addition, SDM version 1.2 has provided feedback to the forthcoming Complete Site Investigation phase (CSI) in terms of additional data needs to aid in reducing SDM uncertainty.

In order to assess uncertainty and confidence in the Site Descriptive Modelling work, procedures (protocols) have been developed. The protocols aim at identifying and quantifying uncertainty in the descriptive models by exploring various origins of uncertainty for the different modelling steps. Less emphasis is put on the importance of the uncertainties, since such an assessment could strictly only be done by the users of the SDM, i.e. it is part of the repository design and safety assessment work.

The protocols are formed as tables with questions to address. These questions concern: i) understanding and use of primary site data, as well as, accuracy and bias in these data; ii) uncertainties in the models, their cause, the potential for alternative interpretations and further site characterisation activities that would reduce uncertainty; iii) consistency between the different discipline model interpretations, iv) consistency with understanding of past site-specific evolution from 2000 million years to the Quaternary and during the Quaternary period, respectively, and v) comparison with previous model versions. For a given version of the SDM, the experts involved in the modelling work within each discipline, i.e. geology, rock mechanics, thermal properties,

hydrogeology, hydrogeochemistry, transport and surface system, first answer these questions. The answers are subsequently assessed and revised in a workshop where these experts from all different disciplines and also members of the site investigation team participate.

The protocols developed have been utilised in the versions 1.1 and 1.2 of the SDM for the Forsmark area and the Simpevarp subarea and the resulting tables with all answers are included in the SDM reports. The assessment of the Forsmark model version 1.2 showed that inaccuracy and biases in data were understood and accounted for in the subsequent modelling. Concerning model uncertainties it was concluded that many of the uncertainties were quantified or explored as alternatives as compared with the preceding model version 1.1, and that additional data needs to reduce uncertainties had been identified in planning of the CSI programme. One of the identified uncertainties in the version 1.2 geological description concerns the occurrence and geometry of deformation zones outside the potential repository volume. This uncertainty was illustrated by formulating alternative models, which were explored in the SDM hydrogeological modelling combined with various assumptions on the location of boundaries and the uncertainty in the transmissivity distribution in the deformation zones. Simulation results suggested that the groundwater flow inside the potential repository volume predominantly is determined by the location, geometry and hydraulic properties of the deformation zones inside this rock volume, whereas alternative descriptions of these zones outside the potential repository volume have little impact on flow inside this volume. From this it was concluded that it is important to resolve the uncertainties associated with the occurrence, geometry and properties of the deformation zones in the repository volume, whereas the corresponding uncertainties in the regional volume outside the repository volume are of no importance for the repository design but may impact the endpoints for migration paths from the repository. Therefore this uncertainty was propagated to the safety assessment work for further analyses of its importance. Additional field investigations to resolve uncertainties in the occurrence, geometry and properties of deformation zones inside the repository volume, such as the excavation and detailed mapping of representative lineaments and mapping and hydrogeological tests in new boreholes, are included in the CSI programme.

The assessment of consistency between disciplines showed that interactions between disciplines that are judged to be important also to a large extent were considered in the modelling, but further improvements in this context were also identified. In general, the Forsmark SDM version 1.2 was found to be consistent with the current understanding of past evolution. Finally, it was concluded that there were considerable developments in the version 1.2 as compared with version 1.1 and that the main reason for this was the substantial increase in site-specific data. The current understanding of the site was primarily confirmed by the outcome of model version 1.2, with increased confidence in the site description. For example, much more sub-surface data implied only minor changes in the lithological description as compared with model version 1.1. In addition, enhanced confidence in rock mechanics and thermal properties was achieved since analyses and modelling, based on a larger data set, confirmed the ranges obtained in model version 1.1

Applying the developed protocols has proved to be an efficient means of uncertainty and confidence assessment. The uncertainties, their cause, and suggested means of reducing uncertainties get documented. Furthermore, applying the protocols and the connected workshops have proven to be an excellent forum for overall cross-discipline integration and to provide insights to the modelling teams on what their uncertainties are and which of these uncertainties could affect other users. These assessments also give direct suggestions for how to continue the on-going site investigation work.

At the current state of site descriptive modelling it is also clear that there are many uncertainties. Some of these uncertainties remain un-quantified and several alternative hypotheses are still left as hypotheses. More data will allow for further quantification and may also reduce many of these uncertainties. However, it will also be important to use feedback from the users of the Site Descriptive

Model, i.e. Rock Engineering and Safety Assessment, on which of these uncertainties really require additional efforts. Such feedback is also expected from the preliminary design work and the Preliminary Safety Assessments to be conducted during 2005.

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