



ENTRY 2003

**- The International Workshop on Reliable Performance Assessment
through Laboratory Experiments and Ground Surface Investigations -**

10th Anniversary of ENTRY



March, 2004

Japan Nuclear Cycle Development Institute
Tokai Works

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ENTRY 2003
- The International Workshop on Reliable Performance Assessment through Laboratory
Experiments and Ground Surface Investigations -
10th Anniversary of ENTRY
(Meeting Document)

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Abstract

To commemorate the 10th anniversary of the ENTRY, a laboratory in JNC Tokai for R&D in the field of geological disposal of radioactive waste, an international workshop was held in JNC Tokai, during the term of Sept 22 to 24, 2003. A technical tour for the Horonobe Underground Research Laboratory site was also done before the workshop, on October 20 to 21, to deepen understanding the background of discussion in the workshop.

The workshop contained two sessions. The topic of each session was

1. long-term transition of the near-field and
2. cooperation among the performance assessment, in-situ experiment, and laboratory experiment, respectively.

In the session 1, we mainly discussed the thermal-hydrological-mechanical-chemical (THMC) coupled processes for the near-field performance assessment, especially focusing on chemical degradation effects by cement materials and the status of mechanistic understanding radionuclide migration. Silicate dissolution kinetic model, including smectite dissolution in a hyper alkaline solution, was also discussed. Then, we discussed a relevant linkage among laboratory experiments, model (simulation experiment) and database development, in-situ experiment and natural analogue.

In the session 2, we discussed 1) methodology for understanding the site based on the surface and boreholes investigations, 2) identification of remained uncertainty after the surface and boreholes investigations, 3) the critical measurement at the surface and boreholes investigations, 4) feedback items from performance assessment to site characterization and 5) required data besides the site investigation.

This report contains the minutes of discussion in the workshop. Presented materials were also appended with permission from the speakers.

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ENTRY 2003

- 室内試験と地表調査による信頼性ある性能評価に関する国際ワークショップ -
エントリー 10 周年を記念して
(会議報告)

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要 旨

サイクル機構東海事業所における、地層処分のための研究開発施設であるエントリーの創立 10 周年を記念して、2003 年 9 月 22 から 24 日にかけて国際ワークショップを開催した。また、このワークショップでの議論の背景について前もって理解を深めておくために、9 月 20 から 21 日にかけて、幌延深地層研究センターへのテクニカルツアーを実施した。

このワークショップは主に 2 つのセッションから構成され、それぞれのトピックは、

1. ニアフィールドの長期変遷
2. 性能評価、原位置試験、室内試験の間の協力であった。

セッション 1 では、ニアフィールドの性能評価のための熱-水-応力-化学連成プロセスについて、特に、セメント材料による化学的な劣化と核種移行のメカニズム理解の現状に焦点を当てて議論した。高アルカリ性溶液中でのスメクタイトの溶解を含めて、珪酸塩の溶解速度モデルも議論された。また、室内試験、モデル（シミュレーション）実験、データベース開発、原位置試験とナチュラルアナログ研究の間の適切な関係についても議論した。

セッション 2 では、1) 地表調査及びボアホール調査に基づくサイト理解のための方法論、2) 地表調査及びボアホール調査後に残った不確実性の同定、3) 地表調査及びボアホール調査での不可欠な測定、4) 性能評価からサイト特性へのフィードバック項目、さらに 5) サイト調査以外から求められるデータについて議論した。

この報告書は主に本ワークショップの議事録を取りまとめたものである。また、ワークショップにて発表された資料については発表者の許可を得て添付した。

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INTRODUCTION

The engineering scale test and research facility (ENTRY) in JNC Tokai, has been carried the principal role on R&D program for the geological disposal of radioactive waste in Japan since the establishment, on October of 1993. To commemorate the 10th anniversary of ENTRY, an international workshop was held in the ENTRY during the term of October 22 to 24, 2003. First, overall lecture was given by H. Ishikawa (JNC Tokai) to make clear the aim of the meeting and to explain surroundings of JNC in the HLW disposal project in Japan. Invitation lectures were then given by Prof. H. Ohmoto (Penn State Univ.) and by Dr. A. Hautojärvi (POSIVA OY).

The aim of the workshop is to obtain suggestions to studies on (1) long-term behavior of the near-field and radionuclide migration mechanism and (2) the level of understanding the site with surface-based and borehole investigations and possible linkage with performance assessment. In the workshop these topics were discussed in the session 1 and 2. In consideration of the aim, we chose 'ENTRY 2003' and 'The international workshop on reliable performance assessment through laboratory experiments and ground surface investigations', as the title and subtitle of the workshop, respectively.

This report contains minutes of discussions with presented materials in the workshop. The program and participants were also noted.

WORKSHOP

Agenda

The International Workshop 'ENTRY 2003' in JNC Tokai October 22 - 24, 2003

General Session (In the Conference Room, 4th Floor of ENTRY)

9:00

Opening address

(H.Ishikawa, JNC)

9:05

Outline of our activities and aim of the Workshop

(H.Ishikawa, JNC)

9:40

Invitation lectures

(Chair: Y.Miyamoto, JNC)

9:40 - 10:40

- Dissolution Kinetics of Smectite and Other Aluminum Silicates in High Alkaline Solutions

(Prof. H. Ohmoto, The Pennsylvania State University, USA)

10:40 - 11:40

- Site Selection, Current Activities and Plans for Future in the Finnish Spent Nuclear Fuel Disposal Programme

(Dr. A. Hautojarvi, POSIVA OY, Finland)

11:40

Notice from the Secretariat

11:45

Facility Tour (ENTRY and overview of 'QUALITY'; a laboratory for radio nuclides migration experiment)

12:30

Lunch

12:30

Leave for JNC Guest House and 2nd Cafeteria

Session I
Long-Term Behavior of the Near-Field
and Radionuclide Migration Mechanism

(In the Meeting Room 301 - 302, 3rd Floor of ENTRY)

Session I October 22 (Wednesday)

13:40

Introduction

(M. Yui, JNC)

14:30

Long-Term Behavior of the Near-Field (1)

Chair: A. Kobayashi (The Kyoto Univ.)

14:30 - 15:20

- Experiences in THM Modeling of Engineered Barriers in Field-Scale Tests at the Canadian Underground Research Laboratory
(D. Dixon, AECL)

15:20 - 15:50

Coffee Break

15:50 - 16:40

- Status of Coupled Process Model Development by Using Prototype Repository Project
(C. Svemar and P. Sellin, SKB)

16:40 - 17:30

- Integrating Thermal, Hydrological and Geochemical Systems to Develop Assessment and Monitoring Strategies
(J. Gansemer, LLNL)

17:30 - 18:00

- Question/Discussion on THM/THC modeling
(All Participants)

18:30

Leave for the JNC Guest House

19:00

Welcome Party Hosted by JNC (JNC Guest House)

21:00

Leave for the Hotel Crystal Plaza

Session I October 23 (Thursday)

8:30

Leave the Hotel Crystal Plaza

9:00

Long-Term Behavior of the Near-Field (2)

Chair: Y. Ohnishi (The Kyoto Univ.)

9:00 - 9:50

- Modeling of Coupled Thermo-Hydro-Chemical (THC) Processes and Rock-Fluid Interactions at the Proposed Nuclear Waste Repository at Yucca Mountain, Nevada
(*N. Spycher, LBNL*)

9:50 - 10:20

Coffee Break

10:20 - 11:10

- Status of a Research Program for Numerical Experiments on the Coupled Thermo Hydro Mechanical and Chemical Processes in the Near-Field of a High-Level Radioactive Waste Repository
(*A. Ito, JNC*)

11:20 - 12:00

- Development of Low Alkaline Cement by JNC
(*Y. Kurihara, JNC*)

12:00 - 13:30

Lunch

13:30

Long-Term Behavior of the Near-Field (3)

Chair: M. Yui (JNC)

13:30 - 14:20

- Cement Degradation: Effects on Bentonite and Rock
(*J. Krumhansl, SNL*)

14:20 - 15:10

- Stability of Bentonites and Formation of Secondary Minerals under Hyperalkaline Condition
(*T. Sato, The Kanazawa Univ.*)

15:10 - 15:40

Coffee Break

15:40

Radionuclide Migration Mechanism

Chair: M. Yui (JNC)

15:40 - 16:30

- Understanding and Thermodynamic Modeling of Radionuclide Sorption on Bentonite and Rocks: Recent Progress and Challenges
(*M. Ochs, BMG*)

16:30 - 17:30

- Discussion on the State-of-the-Art for Long-Term Prediction
(*All Participants*)

18:00

Leave for the Hotel Crystal Plaza

Session I October 24 (Friday)

8:30

Leave the Hotel Crystal Plaza

9:00

Long-Term Behavior of the Near-Field (4)

Chair: M. Yui (JNC)

9:00 - 9:50

- HMC Model Development for TRU Waste Repository

(M. Mihara, JNC)

9:50 - 10:20

Coffee Break

10:20

Discussion on Important Items and Future Direction of Lab., In-situ, Modeling and Databases

Chair: M. Yui (JNC)

10:20 - 12:00

Discussion Points

- Approach for understanding long-term behavior
- Limitation of laboratory, in-situ measurements and natural analogue
- How to obtain confidence in prediction of long-term behavior
- Scenario analysis to be replaced by mechanistic modeling
- Reliability of THMC database (kinetic, thermodynamic database, etc)
- Reliability of numerical experiments
- What's the concerted actions for the long-term behavior prediction / assessment

(All Participants)

12:00 - 13:00

Lunch

13:00 - 14:00 (In the Conference Room, 4th Floor of ENTRY)

Wrap Up

Chairs: M. Yui and M. Uchida (JNC)

- Introduction of summaries of the session I and of II
- Discussions *(All Participants)*

14:00 - 14:40

Facility tour for person who wants ('Inside QUALITY')

13:50 and 15:20

JNC Bus Leaves for the Katsuta Station of JR Railway

Session II
Feedback from Performance Assessment to Site Characterization
Program in the Stage of Ground Surface Investigation

(In the Conference Room, 4th floor of ENTRY)

Session II October 22 (Wednesday)

13:30

Feedback from Performance Assessment to Site Characterization Program in the Stage of Ground Surface Investigation

-Case Histories-

Introduce Questionnaire 1&2

What are current national approaches to Initial Site Investigation (ISI).

Chair: M. Uchida, Co-chair: M. Nishigaki

- Introduction, objectives of workshop, Approval of agenda. (M. Uchida)
- Overview of Questionnaire 1&2 (M. Uchida)
- Discussion (All Participants)

-Discussion on Topics-

14:45

Background and ISI Objectives

What are the program goals for ISI?

Chair: T. Doe, Co-Chair: M. Nishigaki

- Objectives/goals of ISI and desired output from ISI. (T. Doe and all)

15:30

Geosphere conceptual model, PA model and uncertainty

At what point in measurements and analysis do conceptual breakthroughs occur?

Which uncertainty can be reduced and how large uncertainty will remain at the end of ISI?

Chair: A. Strom, Co-Chair: M. Nishigaki

- What level of details do you aim at for modeling (conceptual, numerical, PA) as the result of ISI? (A. Hautojärvi, S. McKenna)
- Uncertainties -- which can be reduced, major breakthroughs, and how large at end of ISI? (A. Hautojärvi, S. McKenna)

19:00

Welcome Party Hosted by JNC (JNC guest house)

Session II October 23(Thursday)

9:00

Feedback from Performance Assessment to Site Characterization Program in the Stage of Ground Surface Investigation

-Discussion on Topics- Continued

Geosphere conceptual model, PA model and Uncertainty

At what point in measurements and analysis do conceptual breakthroughs occur?

Which uncertainty can be reduced and how large uncertainty will remain at the end of ISI?

Chair: A.Strom, Co-Chair: H. Tosaka

- Uncertainties – which can be reduced, major breakthroughs, and how large at end of ISI? Continued (A. Hautojärvi, S. McKenna) --continued

9:45

Chair: W. Darshowitz, Co-Chair: H. Tosaka

- Modeling issues: local scale model, calibration, boundary conditions, DFN, Continuum (W. Darshowitz)
- What are roles for conventional modeling (e.g. groundwater transport) and PA and how do these feedback with field activities? (A. Strom)

Lunch (Box Lunch in ENTRY)

13:00

How we should study geosphere during ISI?

What information should support the ISI goals?

Chair: T. Doe, B. Frieg, Co-Chair: H. Tosaka

- Accounting for heterogeneity – needs in different disciplines (geology, hydrogeology, geophysics, geochemistry, rock mechanics) and reasonable expectations for accuracy, requirements at each scale, optimizing borehole strategies (objectives, location etc.) (R. Munier)
- What are the critical measurements? (e.g. large scale pumping tests, tracer tests) (B. Frieg)
- How can the investigation methods be improved to reduce uncertainty? (Or are there novel methods to reduce uncertainty.) (K. Karasaki)
- How can investigation programs be designed to optimize uncertainty reduction? (T. Doe)
- How are data and conceptual models from other sites (including URL's) used? Does information from generic sites reduce ISI characterization needs (for retention parameters for example) (B. Frieg)

16:30

Endpoint: What are the program goals of ISI? How does one decide the goals are met? How does one assure program goals are achievable?

Chair: A. Hautojärvi, Co-Chair: H. Tosaka (R. Munier, T. Doe)

Session II October 24(Friday)

9:00

Feedback from Performance Assessment to Site Characterization Program in the Stage of Ground Surface Investigation

Summary: Collective view on the ISI (Compilation of Questionnaire 2 answers)

Chair: T. Doe

- Compile goals, expected events, SI methods, level of details of GCM and PA, uncertainty, information to be used besides in-situ data, feedback. Produce compiled questionnaire 2 answers into 2 versions (one for crystalline rock and the other for sedimentary rocks).(Discussion, All Participants)
- Future Cooperation and Information Exchange (M. Uchida)

Lunch (Box Lunch in ENTRY)

Wrap up

(In the Conference Room, 4th floor of ENTRY)

13:00

(Chairs: M.Yui and M.Uchida)

Introduction of summaries of the session I and of II

Discussions

14:00

Facility tour for person who wants ('QUALITY')

13:50 and 15:20

JNC Bus Leaves for the Katsuta Station of JR Railway

Participants

Session1

Hiroshi Ohmoto	Pennsylvania State University
James Gansemer	Lawrence Livermore National Laboratory
Nicolas Spycher	Lawrence Berkeley National Laboratory
James Krumhansl	Sandia National Laboratory
Michael Ochs	BMG Engineering Ltd.
David Dixon	Atomic Energy of Canada Ltd.
Patrik Sellin	Swedish Nuclear Fuel and Waste Management Co.
Christer Svemar	Swedish Nuclear Fuel and Waste Management Co.
Min-Hoon Baik	Korea Atomic Energy Research Institute
Akira Kobayashi	Kyoto University
Tetsuji Yamaguchi	Japan Atomic Energy Research Institute
Mayumi Takazawa	Japan Atomic Energy Research Institute
Kazuhiko Yukawa	Japan Atomic Energy Research Institute
Atsushi Neyama	Computer Software Development Co., Ltd.
Hesham Nasif	Computer Software Development Co., Ltd.
Yoshinao Ishihara	Mitsubishi Heavy Industries Ltd.
Sinzo Ueta	Mitsubishi Materials Corp.
Masakazu Chijimatsu	Hazama Corp.
Yumiko Watanabe	Pennsylvania State University

Session2

Aimo Hautajarvi	POSIVA OY
Sean McKenna	Sandia National Laboratory (SNL)
Anders Ström	Swedish Nuclear Fuel and Waste Management Company (SKB)
Raymond Munier	Swedish Nuclear Fuel and Waste Management Company (SKB)
Kenzi Karasaki	Lawrence Berkeley National Laboratory (LBNL)
William Dershowitz	Golder Associates Inc.
Thomas Doe	Institut Nationale Polytechnique de Lorraine Nancy France (ANDRA)
Bernd Frieg	Swiss National Cooperative for the Disposal of Radioactive Waste (Nagra)
Istvan Szucs	Public Agency for Radioactive Waste Management (PURAM)
Yongje Kim	Korea Institute of Geoscience and Mineral Resources (KIGAM)
Chang-Ha Ryu	Korea Institute of Geoscience and Mineral Resources (KIGAM)
Makoto Nishigaki	Okayama University
Hiroyuki Tosaka	University of Tokyo
Hideo Kimura	Japan Atomic Energy Research Institute
Hiroyuki Tsuchi	Nuclear Waste Management Organization of Japan (NUMO)
Michito Shimo	Taisei Corp.
Naoto Yoshino	Maeda Corp.
Kenichi Ando	Obayashi Corp.
Koji Kawada	JGI Inc.
Shigeyuki Saito	Mitsubishi Materials Corp.
Kinichiro Kusunose	National Institute of Advanced Industrial Science and Technology (AIST)
Hiroyasu Takase	Quintessa Japan
Masakazu Cijimatsu	Hazama Corp.

Overall Lecture

ENTRY 2003, The International Workshop on Reliable Performance Assessment through Laboratory Experiments and Ground Surface Investigations 10th Anniversary of ENTRY

Hirohisa ISHIKAWA

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ABSTRACT

To commemorate the 10th anniversary of ENTRY, a laboratory for R &D in the field of geological disposal of radioactive waste in JNC Tokai, I planned an international workshop. The aim of the workshop is to discuss and information exchange for topical issues on (1) long-term behavior of the near-field and radionuclide migration mechanism and (2) the level of understanding the site with surface-based and borehole investigations and possible linkage with performance assessment. First, the background of the workshop will be shown. Then, I will shortly introduce Japanese organizations and/or institutes regarding the HLW disposal project and their roles. I will also talk about overviews of Japanese HLW disposal project, JNC's R&D program for the project, R&D in ENTRY and QUALITY (a laboratory for radionuclides migration studies in JNC Tokai), programs and on-going activities in the Horonobe and the Mizunami underground research laboratories. Relations between the studies in laboratory and those in URL will also be briefly discussed.

Invitation Lectures

Dissolution Kinetics of Smectite and Other Aluminum Silicates in High Alkaline Solutions

H.Ohmoto^{1,2}, A.C.Lasaga², Y.Watanabe^{1,2}, K.R.Spangler¹, and G.Kamei³

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ABSTRACT

In the JNC's plan for future underground repositories in Japan, the facilities will be built mostly with concrete, and bentonite (smectite) will be the buffer material surrounding the waste-glass canisters. The water in contact with cement becomes high alkaline (pH≈12-13.5). Previous studies have suggested that the dissolution rate (R) and solubility of aluminosilicates in alkaline solutions generally increase with increasing pH but they may decrease with increasing concentrations of Si and Al in solutions. These suggestions have led JNC to plan the use low-alkaline (pH≈11) cement, which contains high contents of silica gel, for underground facilities in order to enhance the long-term integrity of the buffer material. The main goal of our study is, therefore, to obtain accurate data on the dissolution rates and solubilities of smectite and other aluminosilicates in high alkaline solutions, especially on the effects of pH and Si contents of solutions on R; such data are necessary in order to develop reliable numerical hydrological/geochemical models to assess the long-term stability of underground repositories. We have approached this goal from (i) a critical review of the experimental data reported by previous investigators and (ii) our own experimental studies on long- and short- term dissolution of smectite in alkaline solutions.

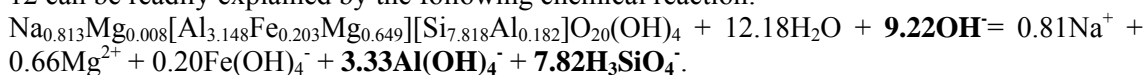
Essentially all the previous experimental studies on dissolution of aluminosilicates were carried out in closed system (e.g. batch reactors). Some experiments (e.g. Cama et al., 2000) were carried out in "flow-through systems", but the long residence time of solutions in the reactors made them hybrids of open- and closed systems. From the change with time in the concentrations of Si (and Al) during dissolution of a mineral ($\Delta m_i/\Delta t$) in a closed system, we may be able to obtain both the long-term dissolution rates (R_{LT}) and the initial dissolution rates (R_{INT}). All the R values reported by previous investigators are R_{LT} . Important characteristics of R_{LT} values of aluminosilicates in alkaline solutions are: (1) The R_{LT} values were typically calculated from the $\Delta m_i/\Delta t$ values at $t > \sim 100$ hrs where the $\Delta m_i/\Delta t$ values were constant; (2) R_{LT} increases with increasing pH: $R_{LT} = k[OH^-]^n$, i.e., $\log R_{LT} = n \log(pH) + c$, where the n typically ranges between 0 and 1.0 and increases with increasing T; (3) At a given pH, R_{LT} typically increases with increasing T; (4) At a given pH and T, R_{LT} decreased with increasing concentrations of Si and Al in solutions: $R_{LT} = k/[Si]^m$; and (5) R_{LT} values are smaller than the dissolution rates calculated from one-day data (R_{1-day}) and $R_{INT} \cdot R_{INT} > R_{1-day} > R_{LT}$.

The R_{LT} values reported by previous investigators are compared at pH=12 and T 25°C for waste glass, basalt glass, nepheline, jadite, albite, forsterite, quartz, corundum, kaolinite, and smectite. The $\log R$ (mol/m²/sec) values ranges from -8.2 for glass to ~11 for kaolinite and smectite; the n value for [OH⁻] ranges from 0 to 1.1. However, when the same minerals were studied by different groups of investigators, the agreements in the R_{LT} and n values are poor. This probably reflects the fact that R_{LT} depends on the mineral/solution ratio. In contrast, the initial dissolution rate (R_{INT}) is independent on the mineral/solution ratio and close to the true

dissolution rate (R_{TRUE}): $R_{\text{apparent}} = R_{\text{TRUE}} - R_{\text{precipitation}}$.

Our experiments were carried out to determine both the R_{LT} and R_{INT} values for smectite at the following conditions: $T=25, 50, \text{ and } 75^\circ\text{C}$; $\text{pH}=8\text{--}13.5$ (pH adjusted by NaOH and HCl); and $\text{SiO}_2(\text{initial})=0, 30, 60, 100, 300, \text{ and } 500 \text{ ppm}$. For short-term experiments (0.5-10 hrs), 120 mg of smectite powder was placed into 40 mL polyethylene centrifuge tubes containing stock solutions pH adjusted by NaOH . The solutions were constantly agitated by shakers. The solutions were separated from the crystals using a high-speed (18,000 rpm) centrifuge for ten minutes and then analyzed for chemical composition (Na , Ca , Fe , Mg , Ti , Al , and Si) using an inductively coupled plasma atomic emission spectrophotometer (ICP-AES). The solid products were analyzed by the X-ray diffraction (XRD) method. Important characteristics of the R_{INT} values are: (1) R_{INT} values are calculated from the $\Delta m_i/\Delta t$ values at $t \approx 0 \text{ hr}$; (2) R_{LT} increases with increasing pH : $R_{\text{LT}} = k[\text{OH}^-]^n$, i.e., $\log R_{\text{LT}} = n \log(\text{pH}) + c$, where the n may be >1 and increases or decreases with increasing T ; (3) At a given pH , R_{LT} typically increases with increasing T ; (4) At a given pH and T , R_{LT} **increases** with increasing concentrations of Si and Al in solutions: $R_{\text{INT}} = k[\text{Si}]^m$. The equilibrium concentrations of Si and Al also increase with increasing $\text{SiO}_2(\text{initial})$ values. Therefore, the smectite dissolution rate in low-alkaline cement environment are not likely to be significantly different from those in Si -poor cement environments.

The kinetics of dissolutions/precipitation of smectite (and other aluminosilicates) in alkaline solutions are found to be greatly influenced by the following parameters: (i) the composition of minerals; (ii) the dependence of concentrations of surface species (AlO^- and SiO^-) of minerals on pH and T ; (iii) the dependence of dominant aqueous species ($\text{Al}(\text{OH})_3^0$, $\text{Al}(\text{OH})_4^-$, H_4SiO_4 , H_3SiO_4^- , $\text{H}_2\text{SiO}_4^{2-}$) on pH and T . For example, the strong dependence on $[\text{OH}^-]$ of the dissolution rates and equilibrium concentrations of Si and Al in the pH range between ~ 9 and ~ 12 can be readily explained by the following chemical reaction:



Important conclusions from this study include: (1) the dissolution rates of smectite in cement and pore fluids are likely to be established within a day; (2) the equilibrium concentrations of smectite in high-silica and high- pH solutions are very large; (3) a combined effects of (1) and (2) is that the buffer material in underground repository may lose its function within short time.

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The main goal of this study is to obtain accurate data on the dissolution rates and solubilities of these minerals in high alkaline solutions, especially on the effects of pH and Si contents of solutions on the rate. His approaches to achieving this goal are 1) a thorough review of experimental data reported by previous investigations and 2) experimental studies on the long- and short-term dissolution of smectite in alkaline solutions.

Based on the results, he suggested that a) the dissolution rate in cement environment (even in low-alkaline cement) are so fast that equilibrium between smectite and pore fluids are likely to be established within a day; b) the equilibrium Si concentrations of smectite in high-silica and high- pH solutions are very large; therefore, c) the buffer material may lose its functionality within a short time after placement in the repository.

The main topic of discussion, after his talk, was about the applicability of TST (Transition State Theory) for smectite dissolution. Dr. Yui asked whether it is possible to incorporate the equilibrium term, based on the TST, for smectite, which may be unstable in solution. Prof.

Ohmoto answered that the dissolution/precipitation model he presented at the meeting is based on basic concepts of TST: some activated compounds are transferred to solution (*i.e.*, dissolution) and the others are transferred back to the mineral surface (*i.e.*, precipitation).

That is, the observed rate of dissolution (R_{obs}) = True dissolution rate (R_{diss}) - precipitation rate (R_{prec}). While $R_{\text{diss}} > R_{\text{prec}}$, dissolution of smectite continues; the solutions are undersaturated with respect to smectite. When $R_{\text{diss}} = R_{\text{prec}}$, it is called a steady state. Neither R_{diss} or R_{prec} becomes zero at a steady state. R_{prec} may be considered as the rate of precipitation of zeolite if zeolite is formed as an alteration product of smectite, or as the rate of precipitation of smectite if no new mineral is formed. In the former case, the steady state may represent the equilibrium condition with zeolite (or smectite); in the latter case, the steady state may represent the equilibrium condition with respect to smectite alone.

Dr. Yui also asked about the effects of compaction which dominates the alteration by transport. Prof. Ohmoto agreed about his comment.

After the workshop, Prof. Ohmoto gave us the following message regarding the smectite dissolution problem, which included the following three figures;

Different Kinds of Dissolution Rates

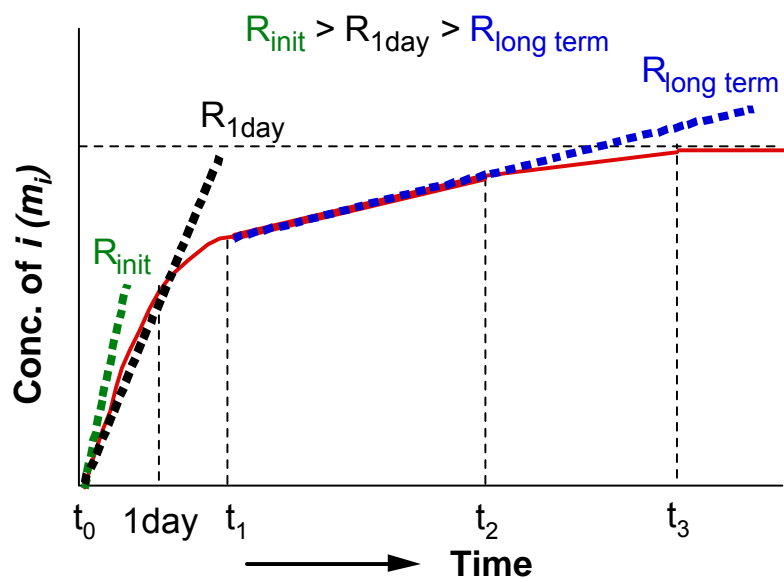


Fig. 1

Fig. 1 schematically illustrates the difference between the initial- and the long-term rates of mineral dissolution in a typical experimental system. The long-term (or steady-state) dissolution rates of aluminosilicates typically range between $\log R_{\text{LT}} = -10$ and -12 at pH = 12 and 25. In contrast, the initial rates (R_{INT}) are typically about two orders of magnitude higher than the long-term rates (R_{LT}). Mineral dissolution in open systems where the dissolved compounds are continuously removed from the systems should be evaluated using the initial rates, rather than the long-term rates. However, the dissolution phenomena in closed systems should be evaluated using both rates: use the initial rates during the early stage of reaction and the long-term rates during the subsequent stage of reaction. But keep in mind that the long-term dissolution rates determined under a unique set of experiments (*e.g.*, water/rock ratio) may not be directly applicable to all systems.

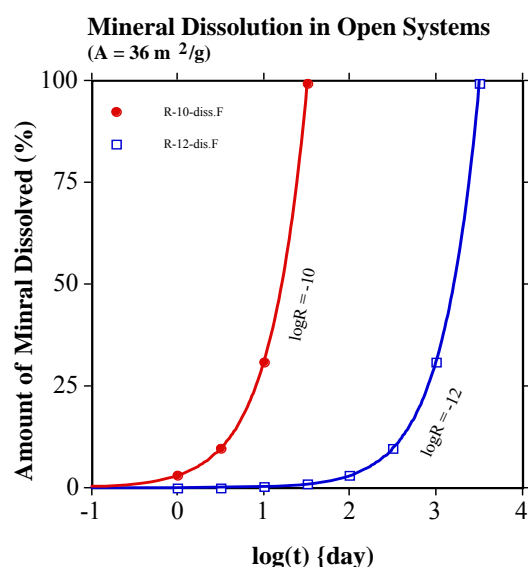


Fig. 2

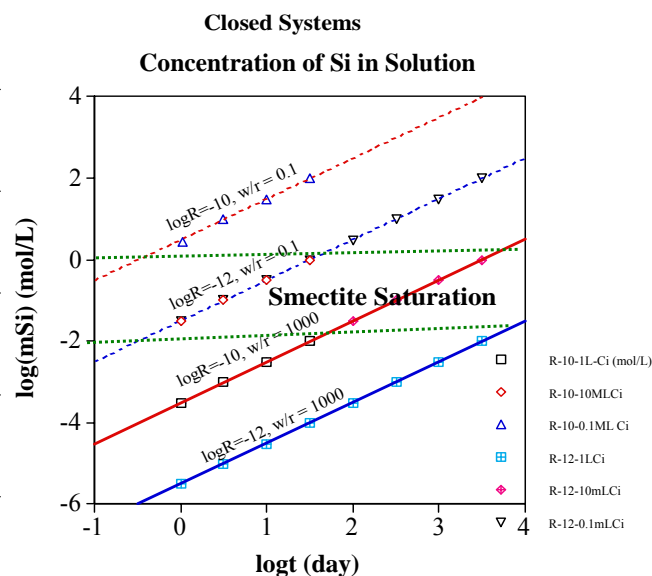


Fig. 3

H, Ohmoto (10/24/03)

Fig. 2 shows the percentage of dissolution of a mineral (*e.g.*, smectite) as a function of time of reaction in an open (or closed) system when the reactive surface area of mineral and dissolution rate remains constant through the entire dissolution period at $36 \text{ m}^2/\text{g}$ and $\log R = -10$ or -12 ($\text{mol}/\text{m}^2/\text{sec}$), respectively. (Note the $\log R_{\text{INT}}$ values can be as high as -8). The entire ranges of the dissolution curves will be valid in open systems where the minerals can completely dissolve away (*i.e.*, 100% dissolution). However, in closed systems, the dissolution curves are valid only where the solutions are undersaturated with the mineral; minerals may or may not be completely dissolved depending on the saturation values. This figure indicates that the mineral will completely dissolve in ~ 30 days at $\log R = -10$ and $\sim 3,000$ days at $\log R = -12$, if the solutions remain undersaturated. In reality, these "dissolution times" may be significantly reduced because the specific surface area of mineral may continue to increase as the mineral grains become smaller during dissolution. An important concept from this figure is that the minerals will dissolve away in relatively short time as long as the solutions are undersaturated.

Fig. 3 shows the change in concentration of Si (moles/L) in water as a function of the water/mineral (w/r) ratio of a **closed system** ($w/r = 1000$ and 0.1) at two different $\log R_{\text{LT}}$ values (red for $\log R_{\text{LT}} = -10$ and blue for $\log R_{\text{LT}} = -12$). Green dotted-lines represent the condition where the solution is in equilibrium with smectite: the $\log m\text{Si}$ values probably lie between -2 and 0 . The blue and red lines will lose the validity beyond the saturation values. Most laboratory experiments, including those by Dr. Sato and by us, were carried out in systems with $w/r \cdot 1000$ (*i.e.*, water dominated conditions). At this w/r ratio and $\log R = -10$, the solution will be saturated with smectite in ~ 50 days. In contrast, the w/r ratios within a compacted buffer zone surrounding a waste canister in repositories would be less than 1. Therefore, the pore fluids in the compacted buffer zone will become saturated with smectite in less than 1 day even when the $\log R_{\text{LT}}$ value was as low as -12 . Note that the dissolution lines in this figure were calculated with an assumption that the $\log R_{\text{LT}}$ values in rock-dominated systems are the same as those in water-dominated systems. The validity of this assumption needs to be evaluated by future experiments. In equilibrium systems, the long-term stability of a buffer zone can be easily computed from the saturation values and the rates of fluid transportation from the buffer zone to the outside. Therefore, in order to quantitatively assess the long-term stability of the buffer (and concrete) in repositories, it is extremely important to experimentally determine the solubility

(equilibrium values) of smectite under a variety of conditions (pH, Si and Al contents, T). Such experiments should be carried out by JNC.

Site selection, current activities and plans for future in Finnish spent nuclear fuel disposal programme

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ABSTRACT

According to the Nuclear Energy Act, all nuclear waste generated in Finland must be handled, stored and permanently disposed of in Finland. The two nuclear power companies, Teollisuuden Voima Oy (TVO) and Fortum Power and Heat Oy, are responsible for the safe management of the waste and for all associated expenses. The power companies have established a joint company, Posiva Oy, to implement the disposal programme for spent fuel, whilst other nuclear wastes are handled and disposed of by the power companies themselves.

The principles of the policy on nuclear waste management were originally defined in a Government decision in 1983. Following the revision of the nuclear energy legislation in 1987, the principles and time schedules for nuclear waste management can be defined by the Ministry of Trade and Industry (MTI), which, has indeed redefined the overall policy in its decisions of 19 March 1991 and 26 September 1995. Most of the policy principles are similar to the 1983 decision and provide a basis for both the practical implementation of nuclear waste management and for the research and development related to the eventual development of a repository for spent fuel.

Posiva's main milestones in the nuclear waste management programme up to the start of the disposal of spent nuclear fuel in 2020 are the following:

- | | |
|------|--|
| 1983 | Government decision and start of site selection studies |
| 1987 | Five areas selected for preliminary site investigations |
| 1993 | Selection of three sites for detailed investigations and one more site (Loviisa) in 1996 |
| 2000 | Application of Decision in Principle and selection of the disposal site (Olkiluoto) |
| 2004 | Start of the construction of ONKALO (Underground Rock Characterisation Facility) |
| 2012 | Application of construction licence for the repository and start of construction |
| 2020 | Application of the operation licence and start of the disposal. |

The site investigations emphasised in the past and will emphasise also in the future the availability and characteristics of suitable rock volumes, "blocks", in different scales. A general trend has been from large scale features towards more fine details. One of the main goals of the underground investigations is to characterise the host rock at the targeted depth and location to reduce uncertainties still remaining after surface investigations and acquire most detailed data for the application of construction licence and later the operation licence.

Before construction of the ONKALO facility the baseline conditions had to be determined as a reference for possible changes and disturbances. Underground characterisation and research programme has been compiled as well. In addition to these reports Posiva has presented to the authorities also a report on possible disturbances and a planning report for monitoring the possible changes and disturbances. Posiva will inform authorities about plans and outcomes on such a level that it can be later possible to include the ONKALO as part of the repository and meet the requirements of a nuclear facility.

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AH began to explain the site selection and current activities in Finland with mentioning that every country has a different procedure for site selection and the Finnish approach should be taken as an example, since it is not necessarily the only approach.

The site is located in the municipality of Eurajoki in Finland. The nearest town is Rauma. Many of the people working at the power plant in Olkiluoto live, in the Eurajoki municipality, and in Rauma. The POSIVA office moved to Olkiluoto more than one year ago.

AH briefly explained the nuclear power plants in Finland. Finland has two sites and four units. The week before, it was decided to construct the fifth unit at Olkiluoto. The capacity is 1600 MW and it should start its operation by 2009. However, the negotiations will continue about the technical details of the reactor. The existing Olkiluoto reactors are boiling water reactors (BWR), the new one will be a PWR and the Loviisa reactors are pressurized water reactors (PWR). The Olkiluoto reactors are operated by TVO, Teollisuuden Voima Oy and the Loviisa reactors are operated by Fortum Power and Heat Oy.

The nuclear waste management scheme of two power plants is such that each plant has its own repositories at the power plant site for the low and intermediate level waste. The repositories for the low and intermediate level waste are constructed typically down to 90- 100 meters in granitic rock. Their layouts and geologic formation are slightly different.

TVO and Fortum jointly established POSIVA, to manage the spent fuel disposal, on behalf of these owners. TVO owns 60% and Fortum owns 40% of the ownership. POSIVA also advise the owners mainly in questions related to the low and intermediate level waste and in a very minor part some other activities. POSIVA has only 40 staffs, although the number was doubled in last couple years. POSIVA extensively uses outside contractors and very closely works together. The annual turnover is 15 million EUROS. The office is located at Olkiluoto.

The structure of the spent fuel management in Finland is that the Government and Ministry of Trade and Industry provide the licenses and the STUK (Radiation and Nuclear Safety Authority) supervises the activities. POSIVA has close contacts with domestic consultants and institutes, as well as the foreign organizations including SKB. POSIVA closely cooperate with SKB on Äspö Hard Rock Laboratory and the encapsulation fabrication methods.

The spent fuel is stored at the interim storage at two power plant sites. Their capacity has been recently expanded to correspond to the demands of the start of the operation of the disposal.

The government decision to dispose of spent nuclear fuel in Finland was made in 1983. Later, in 1996, there was a change in legislation that export or import of nuclear waste in or from Finland is not allowed. By that time, Fortum, that operates the Russian type of reactors VVER-440, returned the fuel to Russia. Therefore, TVO and Fortum decided to establish POSIVA to take all of the waste from that point.

Site selection started with a kind of mapping of potentially possible areas and sites and all the potential municipalities were first asked about their willingness to be a part of the investigations and possibly to allow the final disposal. The areas reduced down to five preliminary site investigation areas by 1987. The safety assessment report was produced in 1992 and presented to safety authorities and the Ministry. This report supported the decision to continue the detailed site investigations on four sites, Eurajoki, Loviisa, Kuhmo and Äänekoski. The

Olkiluoto site in the municipality of Eurajoki was selected in 2000. An underground research facility called ONKALO is now planned to start construction. Construction of the disposal facility will start from 2012 and the final disposal will start in 2020. The repository will be closed sometime later than 2120.

The decision on the final disposal of spent nuclear fuel in Finland was made as follows:

- The safety authority provided a positive statements and opinions,
- The site municipality provided a positive statements and opinions,
- The government made a positive decision complying with the decision in principle, answering the question if this all is for the overall good of the society,
- The parliament approved of the decision in principle by 159:3. The Green Party supported the disposal of the nuclear waste, but they stated that this doesn't mean that they would accept further construction of nuclear power, but the existing fuel had to be disposed of and managed well.

Geologic formation in Finland is basically crystalline rocks and deep geologic disposal concept in Finland considers the blocks. The blocks are determined based on large-scale geological studies on features and lineaments. The first selection of potential sites selected 162 regional blocks. The target areas were further selected and 5 areas were selected for preliminary site investigations. In 1993, four areas were selected for the detailed characterization. The conclusion at that time was that heterogeneity within the site was even more important than the differences between the sites. Therefore, at each site, one could adapt the repository to the existing geology. This is the most important factor considering safety.

The mica gneiss distributes in the Olkiluoto site, and Rapakivi granite formations and sandstone distribute to the east of the site. The Rapakivi granite formations distribute quite near to Olkiluoto and this granite is thought to be dipping down below the Olkiluoto gneisses and the depth at the site is about from 3 to 4 kilometers. Traces of some fluids from Rapakivi granite can be seen in the Olkiluoto gneiss. Crush zones around Olkiluoto were studied based on lineament studies and the area under the sea was studied by mapping the sea-bottom topography and sea-bottom sediments. POSIVA is now concentrating on the block in the central part of the island.

The investigation area is to the east of power plants and is about 1.5 kilometers x 1.8 kilometers. The area is covered with boreholes and other investigations including airborne investigations. Currently, KBS-3 type repository with vertical deposition holes is considered, but the horizontal option is also being studied. The encapsulation plant is not yet decided whether to locate at the site or just next to the interim storage of the spent fuel.

There are two different types of fuels because of two different types of reactors. The major differences are the internal iron support and the length of the canisters. The copper overpack will be used for both types of canisters. Another variation will be studied in next few years, since a third type of reactors will be constructed in Finland.

POSIVA's site investigation at the four sites included geology, geophysics, hydrology, and interpretation and modeling (see OHP#18 for detail). More detailed study from the surface and from the underground will be conducted to confirm the earlier results and to obtain the more detailed data regarding the properties at actual right depth in the bedrock and map the fractures more effectively which can not be always studied with boreholes. The borehole diameters are either 56 mm or 76 mm and the upper part was enlarged to 150 mm to allow installing pumps and different tubings below the ground water table.

A net of GPS stations were established to monitor the possible movement of the block structures and larger scale fracture zones at the site. One permanent station is connected to the Finnish and even International network of GPS stations. All stations are measured in campaigns, twice a year. After ten years of measurements in series, some movement, sub-millimeter scale per year was observed. This corresponds well with the Fenno-Scandian tectonics and bedrock movements and stresses.

The bedrock at Olkiluoto mainly comprises of mica gneiss and partially of tonalite (a slight variant of mica gneiss) and granite. Repository area needed for 2200 canisters is indicated as grayish area (OHP#21).

The geochemistry concept of the bedrock in Olkiluoto is similar to the other sites around the Baltic Sea, like Äspö and Forsmark. More saline waters with salinities up to 80 grams/liter are distributed at deeper part of 800-1000 m deep. The brackish water is distributed above the saline waters. The meteoric water circulates in the most upper parts. The hydrogeochemistry at Olkiluoto represents an evolution and time dependent situation, since the island of Olkiluoto rose up above the sea after the last glaciation and the land uplift continues to push down the saline waters and getting more fresh in the depths of 400 to 500 meters.

Predictive modeling on salinity concentration at Olkiluoto was conducted up to 10000 years A.P. The modeled result evolved corresponding to observations and provided understanding of the present situation. The result after 10000 years indicated more fresh water at 500m deep, where the repository is tentatively indicated.

Possible disturbances caused by excavation of the ONKALO (Underground rock characterization facility) and the repository should be carefully treated, because these will be kept open more than 100 years. Drawdown of groundwater level was calculated for the environmental impact assessment and it indicated that the groundwater table would drop several tens of meters at the site. This calculation didn't take into account possible measures taken to grout the rock. There is an on-going discussion on the use of cement based grouting materials. In order to consider the possible effect of high-alkaline plumes from the grouting materials, we need to look into the effects such that i) The ratio of releasing the calcium hydroxides to the water flows, dilutes the plume by almost two units of pH, by around a factor of 100 and ii) There could exist other sink besides repository and that sink would take the high pH plumes away from the repository. We need to understand the groundwater flow in order to answer for the cement issues and for radionuclide transport issues.

Main activities of POSIVA were to measure the ground water flows and to develop new techniques and instruments to better observe the hydraulic conditions. An example of a device is the PAVE (pressurized water sample) system, which allows to take pressurized water samples at the depths to observe microbes or to observe gas without releasing the gas pressure at the ground surface.

One more issue that POSIVA will present in the future safety assessments is the analysis of potential rock movements and earthquakes. POSIVA has collected the earthquake data and modeled the potential effects of the earthquakes. The result showed that the probability of rock movements of a few centimeters would be extremely low, even after a glacial rebound phase. Therefore, POSIVA thinks that the bedrock is mechanically, chemically, and physically stable and suitable for disposal of nuclear waste in the Finnish bedrock at Olkiluoto.

POSIVA will continue the surface based investigations while constructing ONKALO up to the application of the construction license of the repository in early 2010's. The authorities and their international review team are very keen on understanding the baseline (present situation) prior to start disturbing it due to excavation. POSIVA presented the baseline description report of ONKALO, although no further licenses are required to construct ONKALO. POSIVA has assessed the disturbances and has presented the first version of the underground characterization and research program. POSIVA will present R and D program every three years and the first one by the end of 2003. POSIVA will also present a monitoring plan to monitor potential disturbances.

ONKALO has access tunnel of 1:10 inclination, the main characterization tunnel at a depth of 420m which is the actual repository level and the lower characterization tunnel at the depth of 520m, as well as the ventilation shaft. POSIVA will study the representative bedrock in detail. The actual repository will be constructed next to the characterization facility.

Questions and answers

MU asked the area covered by the spiral access tunnel. AH replied that the spiral tunnel covers approximately 150m x 250m area and this covers 10% of the repository at most. The spiral tunnel is designed to be tight to minimize disturbance, but to get a good picture of the rock structure in advance to verify observations made from the surface boreholes. There is one longer loop to get the features in wider area. The loop is designed taking into account of rock stress and foliation.

MU asked if there will be horizontal holes to cover the repository area. AH replied there will be an inclined holes to cover 200 x 200m area drilled from the depths between 250 and 350m. AH explained that this depth is decided to avoid connections between the repository facilities and the conductive fractures. AH commented that there will be a need to invent some means to satisfy this requirement, such that drill a borehole from the ground surface to -300m and extrapolate the obtained data. Horizontal holes will reveal vertical fracture frequency.

MS asked if the hydraulic boundary condition will be affected by faults or lineaments although Olkiluoto is surrounded by the sea. AH replied that the saline water is being pushed away and causing density change. But, this effect will not be significant and the hydraulic gradient is small due to the flat topography (< 1%). AH pointed out that the salinity profile around the underground facilities will be affected and we need to understand this.

KM commented that Japan also should consider the GPS to monitor the active tectonics and earthquake to ensure the long-term stability of the repository. AH commented that POSIVA has already established a micro-seismic network on the ground surface in addition to the GPS system.

MY asked the construction materials and bentonite. AH replied that the pre-compacted bentonite will be used for the buffer material and the standard backfill material which consists of 30 % of bentonite and 70 % of crushed rock will be used to backfill the KBS-3 tunnels. AH commented that the specification may not be enough to ensure stability for swelling and that further technology has to be incorporated to this problem. MY asked whether POSIVA choose low cost or high performance. AH replied POSIVA will not use 100 % bentonite and the amount of bentonite should be adequate for the purpose of right geochemical requirements. AH commented that POSIVA will use 100 % bentonite buffer for the potential horizontal

deposition tunnels.

MU asked whether the concerned impact is drawdown or altering geochemical conditions. AH replied that drawdown is not a concern, since there are no houses or farms in the vicinity of the site and just the forests. There is a potential geochemical concern: loose buffer would reduce confinement capacity. Also, oxidized condition and CO₂ concentrated water would be concerns. In order to limit the saline water upconing to avoid the effect for the backfill, tunnel inflow should be kept to minimum and grouting becomes important. MU pointed out that tunnel inflow could wash out fracture filling material. AH agreed that it could potentially happen and transmissivity would become high and that this has to be kept in mind.

Session 1

Introduction

- Long-term behavior of the near-field and radionuclide migration mechanism -

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MINUTE

Dr. Yui was the manager of session 1 of ENTRY workshop. There were about 40 participants including 9 guests from overseas, several guests from JAERI, Japanese universities and Japanese commercial companies. Dr. Yui presented an introduction about the theme of Session 1 (Long-term behavior of the near-field (NF) and radionuclide migration mechanism) after self introduction by all the participants.

Understanding the long-term behavior of the NF is very important to increasing confidence in performance assessment (PA). One of the difficulties in predicting the long-term behavior of the NF is the coupling phenomenon of the thermal-hydrological-mechanical-chemical processes called 'THMC'. THMC is a very complicated coupling phenomenon that will happen in the radioactive waste repository. The public wants to know what will happen after repository closure. For example, there is a conceptual evolution model for long-term behavior of a high level radioactive waste (HLW) repository. During the initial 100 year term following repository closure, nothing will happen. 1,000 years after repository closure, mechanical failure of the overpack is assumed to occur due to anaerobic corrosion and the consequent gradual decrease in strength. Groundwater can then come into contact with the glass waste form and radionuclides contained in the wastes can be released. However, even after the passing of 10,000 years, most (*e.g.*, 90%) radionuclides will remain in the engineered barrier. Such a conceptual model helps the public to imagine the long-term behavior of radioactive waste.

PA of geological disposal is carried out based on scenario development, system model development, and comprehensive data. Assessment includes many assumptions according to the various scenarios, but it is needed to predict what would occur in the future after repository closure. Numerical experiments, based on an understanding of complicated phenomena in the NF, such as THMC, reliable basic data, and mechanistic models provide the results for prediction reliability.

Monitoring in the early stages of repository operation and closure can provide confidence in predictions made by mechanistic modeling/numerical experiments of THM or THMC. Chemical aspects might dominate after repository closure. Numerical models validated by monitoring can provide reliable results for repository behavior prediction, an understanding of the implications for simplification of PA, and an understanding of the processes for the public as well for experts.

The principle challenges facing THMC problems are 1) understanding the coupled processes, 2) the limitation of laboratory, *in-situ* experiments and natural analogue, 3) evaluating the status of perturbation analysis/alternative ways (cement effects) and 4) confidence in numerical experiments. The complexity of the phenomena as well as a lack of communication among different areas of studies (*e.g.*, thermal, hydrological, mechanical, chemical, biological *etc.*)

makes predictions of long-term behavior difficult.

All experiments (*i.e.*, laboratory experiments, *in-situ* experiments, natural analogues) have their limitations. For example, relationships between time covered by each experiment and the reliability of the long-term prediction (LTP) are summarized below:

- Normal laboratory experiments might be applied for only a short time and are not relevant for LTP.
- Accelerated laboratory experiments might be applied for a long time period (but still, the period is very limited) but normally are not relevant for LTP due to changes in mechanisms.
- *In-situ* experiments might be applied for a short time and are relevant for heterogeneity, but are not relevant for LTP.
- Natural analogues can be applied for long time periods and are relevant for LTP, but both the period and the relevance are limited.
- Numerical experiments can be applied for long time periods and may be relevant for LTP.

However, a combination of these various experiments allows us to obtain confidence in long-term predictions.

Dr. Yui highlighted the following discussion points from session 1.

- Approach for understanding long-term repository behavior
- Limitation of laboratory experiments, *in-situ* experiments and natural analogues
- How to obtain confidence in predictions of long-term repository behavior
- Scenario analysis to be replaced by mechanistic modeling
- Reliability of mechanistic databases (kinetics, thermodynamics, *etc.*)
- Reliability of numerical experiments
- What is the concerted action for long-term repository behavior, prediction/assessment?

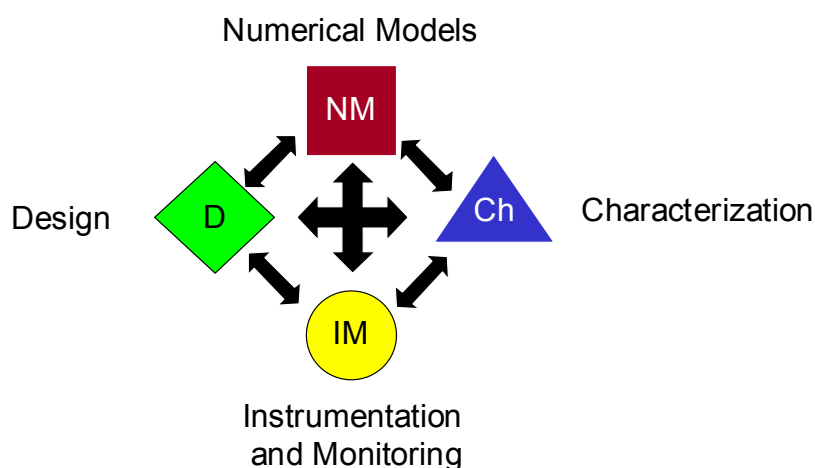
THM Modelling of Engineered Barriers in Field-Scale Tests at the Canadian Underground Research Laboratory

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ABSTRACT

The Canadian Underground Research Laboratory (URL) located near Winnipeg Canada has operated for the past twenty years, providing support to the geoscience and engineering research programs directed towards development of a concept for isolation of Canada's used reactor fuel. A major component of this program has been the design, construction, operation and analysis of large-scale, in situ engineered barriers experiments. Three of these experiments are the Buffer/Container Experiment (BCE), the Isothermal Buffer-Rock-Concrete Plug Interaction Test (Isothermal Test - ITT) and most recently the Tunnel Sealing Experiment (TSX).

In order to define and develop an integrated set of tools to optimize the engineering design of repository sealing systems, input from numerical modelling, seal system characterization and instrumentation/monitoring activities are required (see figure below). These activities are interrelated. Seal system components and materials may be characterized through both bench-scale laboratory and large-scale in situ experiments, such as the BCE, ITT and TSX. At the same time, these tests provide an opportunity to develop instrumentation and monitoring methods and provide data for calibration or validation of numerical models. Numerical models, through back analysis and history matching of experiment monitoring results, can advance our understanding of the behaviour and characteristics of seal system components and materials. Numerical models will ultimately feed into repository engineering design. They are needed to understand the processes going on with in the geologic environment of a used fuel repository and allow prediction of the evolution of the repository under complex Thermal-Hydro-Mechanical-Chemical-Biological conditions.



Engineered barriers experiments were constructed, at full-scale, in a previously undisturbed mass of sparsely fractured granitic rock at the Canadian URL. The BCE and ITT examined the in-floor container emplacement geometry. The movement of groundwater and the development of mechanical and hydraulic stresses in the clay barrier materials and the adjacent rock mass were thoroughly monitored under conditions of no thermal gradient (ITT) and a thermal gradient simulating that induced by a used fuel container (BCE). These experiments were carried out under natural, realistic geologic conditions and allowed for the development of

a comprehensive set of field measurements that could then be used for testing and calibration of numerical models to describe and predict system evolution.

Prior to the operation of the BCE and ITT numerical simulations were conducted using the best-available material properties and parameters for the sealing components and the surrounding rock mass. Comparison of the pre-test predictions and the post-test physical measurements, together with the monitored state during test operation, demonstrated that the thermal evolution of the systems could be predicted reasonably effectively using the existing numerical modelling tools. The hydraulic evolution of the clay mass could be qualitatively predicted by some numerical tools but history-matching was difficult to achieve due to the complex THM processes active within these installations. It was determined that certain materials properties and processes were not well enough understood to allow accurate numerical predictions or history matching to be accomplished. This has led to the development of revised numerical tools that include more complex THM processes to simulate system evolution. In many cases there is still a lack of material property information and understanding of the hydraulic and mechanical interactions between the components of these installations. Conduct of these large-scale simulations, together with ongoing laboratory-based materials properties and process investigations is intended to ultimately refine numerical tools to a point where they can be calibrated against other similar field installations and then be used with confidence for repository evolution predictions.

The TSX, currently operating at the Canadian URL, is a full-scale sealing demonstration that is examining the performance of a concrete-based and a clay-based bulkhead under temperature and hydraulic conditions that might be encountered in an actual repository. These extensively instrumented bulkheads have been monitored over a 5 year period to assess the THM evolution and performance of these materials. Numerical modelling exercises were conducted as part of the planning and design process for the TSX and played a significant role in the ultimate design and operation of this experiment. Numerical modelling exercises conducted prior to and over the course of experiment operation have provided valuable insight into the need for selection of parameters and processes that can affect system performance. Conduct of a field-scale experiment such as the TSX has highlighted some of the limitations of existing numerical models as well as the potential for unexpected physical processes that have yet to be accounted for by numerical simulations. Some of the preliminary results of the THM evolution of the TSX are presented and discussed in the course of this presentation.

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Sealing system components and materials may be characterized through both bench-scale laboratory and large-scale in situ experiments, such as the Buffer/Container Experiment (BCE), the Isothermal Buffer-Rock-Concrete Plug Interaction Test (Isothermal Test "ITT") and the Tunnel Sealing Experiment (TSX). These tests simultaneously provide an opportunity to develop instrumentation and monitoring methods and provide data for calibration or validation of numerical models. Numerical models, through back analysis and history matching of experimental monitoring results, can advance our understanding of the behavior and characteristics of sealing system components and materials. Numerical models will ultimately feed into repository engineering design. They are needed to understand the processes going on in the geologic environment of a used fuel repository and allow prediction of the evolution of the repository under complex Thermal-Hydro-Mechanical-Chemical-Biological conditions.

Some of the preliminary results of the THM evolution of the BCE, ITT and TSX were presented and discussed in the course of this presentation. Key issues of discussions were a) a water saturation mechanism in the compacted clay materials, b) a reliable code to predict the

long-term behavior of THM and c) consideration of chemical behavior in the experiments.

Saturation of compacted bentonite has been observed several years after emplacement, but the saturation mechanism has not yet been well understood because of the structural complexity of the compacted bentonite. Thus, further investigation is needed to understand the saturation mechanism.

There was a discussion about which code was more relevant for the prediction of long-term behavior of THM. Dr. Dixon presented the results of modeling exercises conducted as part of several field-scale experiments conducted by Atomic Energy of Canada. Three coupled codes named TRUCHAM, FLAC and COMPASS were used in these modeling efforts. Depending on the specific application, each code has its limitations and strengths for use in numerical predictions.

The behavior of bentonite altered by high pH solutions from concrete materials has not been well investigated through experimental studies under conditions relevant to a deep geologic repository. For example, there are analytical results for the components of Cl, SO₄, but limited data for Si and Al. Both Si and Al data are perceived as being important from the view point of the effect of concrete materials on bentonite stability, as well as system pH. Therefore, these chemical components should also be analyzed when investigations into concrete-bentonite interaction are undertaken.

Status of coupled process model development by using Prototype Repository Project

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Svensk Kärnbränslehantering AB

ABSTRACT

The Prototype Repository is an international EU-supported project with the objective to investigate the integrated performance of engineered barriers and near-field rock on a full scale in a deep repository-like environment. This is done at 450 m depth in the Äspö Hard Rock Laboratory in granitic rock. The test set-up comprises two sections with 4 canister positions in the inner one and two in the outer. One cast plug separates the inner section from the outer and one the whole test from the other parts of the laboratory, see Fig 1. Important processes are monitored and studied, like heat evolution and distribution, rock mechanics, bentonite saturation, water flow, water chemistry, gas evolution and microbial activities.

A large number of boreholes have been drilled to characterise the rock mass. The instruments in them, many re-installed, will be used for the long-term monitoring of the processes taking place. In addition a large number of instruments have been installed in the buffer, backfill and plugs.

The evolution of the KBS-3 buffer and backfill is being modelled with respect to temperature (T), water migration (H), stress and strain (M), as well as to chemistry (C) and biology (B). Five THM models have been proposed to be used by the individual partners engaged in the study and some of them also include possibilities to add chemical processes in the buffer evolution. One model deals solely with water chemistry. The basis for selection and development of these numerical tools for predicting and evaluating the processes in these engineered barriers is a simplified conceptual model, shown in Figure 2.

A number of physico/chemical events will take place in the maturation of the buffer of which the following are considered to be particularly important:

1. Thermally induced redistribution of the initial porewater.
2. Maturation of the 50 mm thick pellet backfill.
3. Uptake of water from the rock and backfill leading to hydration of the buffer.
4. Expansion of the buffer yielding displacement of the canisters and overlying backfill.
5. Dissolution of buffer minerals and precipitation of chemical compounds in the buffer.

The five proposed EBS model codes are presented below. The large majority of the mathematical expressions is given in /Pusch 2001/.

- *COMPASS (University of Wales)*
- *CODE-BRIGHT (Univeritat Polyitecnica Cataluna) ????*
- *CODE ROCKMECH (BGR)*
- *THAMES (Japan Nuclear Fuel and Waste Management Co – JNC)*
- *ABAQUS (Clay Technology AB)*
- *Chemical model codes PHREEQ-C2 and NETPATH (VTT Finland)*

The work started with selection of the models and identification of their features and parameter requirements. The models were then used for predictive modelling before the six canister units were installed. The result of this modelling is now compared to the actual development, which is represented by data during about two years of observation for the first installed units.



Figure 1. Schematic view of the Prototype Repository with one inner and one outer section.

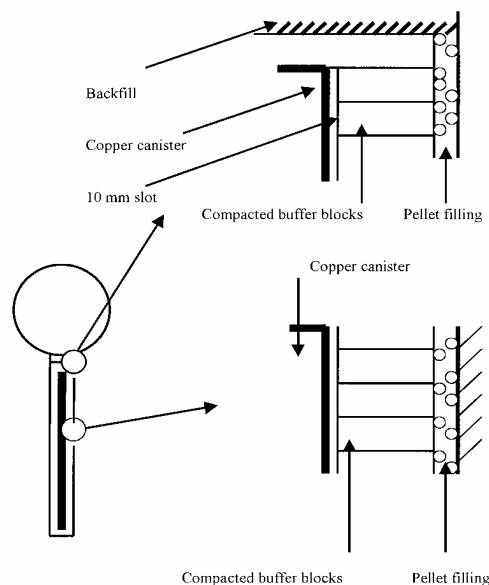


Figure 2. KBS-3 deposition hole with copper-shielded canister embedded in compacted buffer blocks and bentonite pellets filling.

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The Prototype Repository is an international EU-supported project. The objective is to investigate the integrated performance of engineered barriers and near-field rock on a full scale in a simulated deep repository environment. This project has been carried out in a granitic rock at Äspö Hard Rock Laboratory in Sweden.

Important processes are monitored and studied, like heat evolution and distribution, rock mechanics, bentonite saturation, water flow, water chemistry, gas evolution and microbial activities. The evolution of the KBS-3 buffer and backfill is being modelled with respect to temperature (T), water migration (H), stress and strain (M), as well as to chemistry (C) and biology (B). Five THM models have been proposed to be used by the individual partners engaged in the study and some of them also include possibilities to add chemical processes in the buffer evolution. One model deals solely with water chemistry.

Dr. Yui asked what the criterion was for the backfill material that SKB was considering. Dr. Sellin answered that SKB considered the backfill material as a mixture of 30% bentonite and 70% sand. As the backfill material, the applicability of bentonite pellet in the saline type groundwater was confirmed when the pellet was of high density (2.0 g/cm^3). Dr. Yui wondered whether the excavated disturbed zone (EDZ) might be a pathway of radionuclide migration or if the pore spaces among the backfill materials might be the critical path. Dr. Sellin suggested that it might depend on the drift's excavation method. For example, if the drifts were excavated by TBM (Tunnel Boring Machine) method, the zone of EDZ may be reduced and it may not be a critical path for migration of radionuclides. Finally, Dr. Yui questioned the sampling method of pore water in the bentonite and the method of pH measurement. Dr. Sellin explained how to obtain the pore water samples and measure the pH values in the bentonite. The pore water samples were taken from the point making contact with bentonite, using a filter. The pH value of the pore water was analyzed after the bentonite sample was taken out. A measured pH value could be modeled by considering the effects of cooling and degassing after the bentonite sampling.

After the presentation by Dr. Sellin, several issues of discussion about the coupling model of THMC were presented by Dr. Svemer and discussed. The main discussion point was the saturation process in compacted bentonite. Complete saturation in compacted bentonite was doubted because of the complexity of bentonite structure, two-phase flow, and the existence of H_2 and N_2 gases. As the result of the discussion, it was recognized that the saturation process in compacted bentonite was not well understood and further research is needed.

Integrating Thermal, Hydrological and Geochemical Systems to Develop Assessment and Monitoring Strategies

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ABSTRACT

Monitoring processes in subsurface engineered facilities is an important means of evaluating the long-term health of environmental systems, and has become an integral part of high-level nuclear waste repository efforts. Monitoring such systems, however, may be affected by changes in climate that slowly propagate through subsurface systems. We describe in this paper the use of NUFT-C, a reactive transport simulator designed to run on a high performance, massively parallel computer, to quantitatively compare the evolution of a deep geological system with changes expected from an engineered high level nuclear waste repository. The results suggest that the impacts from waste emplacement are, in some instances, similar to those that would be observed as a result of climate change, while others are distinguishable from evolution of the natural system. Such simulations facilitate design of long-term monitoring programs that take account of these complex effects. The results emphasize the importance of developing long-term baseline measurements and control sites, in order to enhance confidence in interpretations of complexly evolving data sets that will be obtained from multi-decade monitoring efforts.

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Glassley, W.E., Nitao, J.J., Grant, C.W., (2003) *J. Contam. Hydrol.*, **62-63**,495-507.

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Monitoring processes have become an integral part of high-level radioactive waste repository. Monitoring may be affected by climate changes that slowly propagate through the subsurface system. Assessing the long-term performance of a subsurface repository would ideally consider fully coupled thermal-hydrological-geochemical-mechanical effects, which effects are realistically measurable and suitable for monitoring, spatial resolution to establish most efficient monitoring strategy, and how to distinguish between natural (climate) and repository-induced changes.

This study presents the results of simulation using NUFT-C to compare quantitatively the impacts from climate change with repository-induced changes. The results suggest that the impacts of repository perturbation are similar to that from a result of climate change, while others are distinguishable from evolution of the natural system. Comparison of the repository perturbation with the natural evolution of the pore waters suggests that monitoring efforts must consider sub-meter scale variability, that the magnitude of variability differs with local heat output, that long-term monitoring must consider 3-D effects, and that water chemistry can be a sensitive detector but only for certain species. The simulation results facilitate design of long-term monitoring programs that take into account these complex effects.

Dr. Yui asked about the database used in the simulation (*i.e.*, how to review and develop the database) and the reason why two systems were considered in the simulations. Dr. Gansemer answered that there was a database developing group for the Yucca Mountain Project (YMP) and the database for YMP was used for this study. The two systems were considered to

distinguish the effects between climate and repository-induced changes.

Prof. Ohmoto questioned the origin of HCO_3 in the water. It could be derived from rain water and/or minerals in the rock mass. Carbonate concentrations may change either climate changes or temperature changes or both. Dr. Spycher suggested that the origin of HCO_3 might be the dissolved $\text{CO}_2(g)$ in this study.

Finally, Dr. Yui asked the future direction of this study (*i.e.*, virtual repository, generic simulation, specific simulation for YMP *etc.*). Dr. Gansemer said that it would be focused on the sensitivity analysis to identify the key factor to affect the simulation results.

Question/Discussion on THM/THC modeling

All Participants

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After all the presentations on the 22nd of October in Session 1, the difficulties of THMC coupling were discussed. Several opinions from the discussion are summarized below.

Dr. Yui suggested that the THM coupling based on the experiences in Canada (AECL) and Sweden (SKB) are OK but the coupling of chemistry needed more work. Prof. Ohmoto added the comment that there appeared to be a lack of chemists' interaction during the planning and design phases of experiments.

The zone of chemical effects in the repository might be small but the effects have a long-term influence. Such long-term effects are difficult to confirm by experiments. It is very difficult to extract the chemical effects from multi-process phenomena like THMC due to the small effects during the short-term experiment.

Dr. Dixon commented that in his experience, chemical effects have been included in the experimental planning and design process but that since chemical effects are less well defined, they are often pushed into the background. Also microbiological and biochemical processes are beginning to be seen as important and probably should begin to be included in the discussion.

Dr. Yui insisted on the importance of *in-situ* measurement of pH and pore water chemistry in compacted bentonite. Prof. Ohmoto put forth a question about how to determine the chemistry that might be found in smectite and wondered if it might be possible to put a quantity in a solution, spin it in a centrifuge, and then perform some type of assay. Dr. Krumhansl verified that it could be done and offered that good information about pore water in compacted bentonite could be found in the literature from the research of marine sediment.

Dr. Sellin commented that it would help the overall repository analysis to determine what and when it is possible to couple together processes. Dr. Yui answered that the early stage of repository might be dominated by THM phenomena. After the heat generation caused by waste packages decrease, HM phenomena will be the main process. Later chemical process will be important.

Finally, Dr. Yui proposed a theme of discussion for the next day. What is the state-of-the-art for long-term prediction? He also required the guest participants to show their personal ideas and/or plans about how we should present the state-of-the-art of THM and/or THMC.

Modeling of Coupled THC Processes and Rock-Fluid Interactions at the Proposed Nuclear-Waste Repository at Yucca Mountain, Nevada

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ABSTRACT

Assessing the long-term performance of geologic nuclear waste repositories necessitates evaluating the effects of coupled thermal, hydrological, and chemical (THC) processes for time periods lasting thousands of years. To reach this goal and gain confidence in our predictive ability, an integrated modeling approach was developed consisting of: (1) process model development, (2) conceptual and numerical model development, (3) design of field and laboratory tests for model validation, (4) predictive analyses of test results, (5) test implementation, (6) comparisons of experimental results with predictive analyses, (7) model refinement and validation, and (8) model implementation for long-term predictive analyses. As part of this approach, an existing reactive transport numerical simulator (TOUGHREACT; Xu and Pruess, 2001) was refined and validated for applications specific to nuclear waste disposal (e.g., Xu et al., 2001; Spycher et al., 2003a). The simulator considers water, vapor, air, and heat transport; reactive gas, mineral, and aqueous phases; porosity-permeability-capillary pressure coupling; and dual (fracture/matrix) permeability. The simulator and modeling approach were applied to the proposed high-level nuclear waste repository at Yucca Mountain, Nevada, to evaluate the chemistry of waters that could seep into drifts and the effect of water-gas-rock interactions on the long-term hydrological behavior around the repository.

The proposed repository at Yucca Mountain is located in fractured, welded volcanic tuffs, several hundred meters above the regional water table. The fracture permeability (10^{-13} – 10^{-12} m²) is several orders of magnitude higher than the rock matrix permeability (10^{-17} – 10^{-19} m²). In these unsaturated tuffs, water is held mostly in pores of the rock matrix (liquid saturation ~0.8–0.9). Upon waste emplacement and subsequent heating (due to radioactive decay), the matrix water would boil and travel as vapor in the fractures. In cooler regions above the repository, it would condense and drain back towards the boiling zone. This continuous boiling and refluxing of water is anticipated to induce mineral dissolution and precipitation, and alter the chemical composition of pore waters surrounding emplacement drifts.

These coupled processes were investigated using underground thermal tests and laboratory experiments. THC simulations of the Drift Scale Test (Sonnenthal, 2003; Xu et al., 2001) and of plug-flow reactor and fracture sealing experiments (Kneafsey et al., 2001; Dobson et al., 2003) provided the basis for model validation. Long-term (100,000 years) predictive analyses were then carried out to evaluate the effects of coupled THC

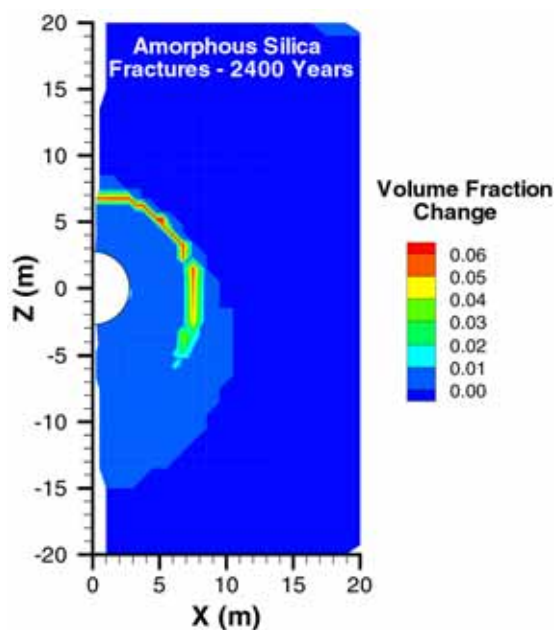


Figure 1. Predicted silica precipitation

processes around a typical nuclear-waste emplacement drift (Spycher et al., 2003a and b).

The long-term simulations indicate that fracture water in the area of highest liquid saturation above the modeled drift undergoes three distinct stages. First, dilution occurs as matrix water boils and condenses in fractures (from ~50 to 150 years). Because of capillary forces, the boiling front in the matrix stops expanding earlier than in fractures. Evaporative concentration then takes place (from ~150 to 600 years) under near-constant (boiling) temperatures as continuous boiling, condensation and refluxing take place in fractures. Finally, water compositions slowly return to original concentrations as the boiling front collapses towards the drift. While liquid saturations are significantly larger than residual, no extreme pH or salinity values are predicted. The dominant mineral to precipitate is amorphous silica, which forms in a thin zone within fractures around the drift (Figure 1) as the result of evaporative concentration at the boiling front. Depending on initial fracture porosity, this precipitation can lead to permeability reductions sufficient to deflect the bulk of percolating water around the drift. Investigations are under way to assess the model uncertainty and implications for long-term evaluation of repository performance.

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Assessing the long-term performance of geologic nuclear waste repositories requires evaluating

the effects of coupled thermal, hydrological, and chemical (THC) processes for time periods lasting thousands of years. To reach this goal and gain confidence in our predictive ability, an integrated modeling approach was developed consisting of; 1) process model development, 2) conceptual and numerical model development, 3) design of field and laboratory tests for model validation, 4) predictive analyses of test results, 5) test implementation, 6) comparisons of experimental results with predictive analyses, 7) model refinement and validation, and 8) model implementation for long-term predictive analyses. As part of this approach, an existing reactive transport numerical simulator called TOUGHREACT was refined and validated for applications specific to nuclear waste disposal. The simulator considers water, vapor, air, and heat transport; reactive gases, minerals, and aqueous phases; porosity-permeability-capillary pressure coupling; and dual (fracture/matrix) permeability. The simulator and modeling approach were applied to the proposed high-level nuclear waste repository at Yucca Mountain, Nevada, to evaluate the chemistry of waters that could seep into drifts and the effect of water-gas-rock interactions on the long-term hydrological behavior around the repository.

The long-term simulations indicate that fracture water in the area of highest liquid saturation above the modeled drift undergoes three distinct stages. First, dilution occurs as matrix water boils and condenses in fractures (from ~50 to 150 years). Because of capillary forces, the boiling front in the matrix stops expanding earlier than in fractures. Evaporative concentration then takes place (from ~150 to 600 years) under near-constant (boiling) temperatures as continuous boiling, condensation and refluxing take place in the fractures. Finally, water compositions slowly return to original concentrations as the boiling front collapses towards the drift. While liquid saturations are significantly larger than residual, no extreme pH or salinity values are predicted. The dominant mineral to precipitate is amorphous silica, which forms in a thin zone within fractures mostly above the drift as the result of evaporative concentration at the boiling front. Depending on initial fracture porosity, this precipitation can lead to permeability reductions sufficient to deflect the bulk of percolating water around the drift. Investigations are under way to assess the model uncertainty and implications for long-term evaluation of repository performance.

Important issues of discussion in this presentation were a) examples of natural analogues for THC, b) minerals considered in the prediction and c) a linkage between THMC and radionuclide migration models.

Dr. Spycher mentioned a colleague is using Yellowstone as a natural analogue site to test the ability of TOUGHREACT to predict long-term THC effects. The rock types are in general similar to those at Yucca Mountain and permeability and porosity data have been measured such that these data can be used to test the model. However, he emphasized the Yellowstone site is not a true natural analogue for the Yucca Mountain site.

The selection of potential secondary minerals that could form as the result of THC processes is important. The choice of these secondary minerals can affect the result of simulations. For the Yucca Mountain study, the secondary minerals were selected primarily on the basis of field data in existing thermally altered areas, and the results of "batch" reaction-path equilibrium calculations considering a multitude of potential secondary minerals (using the CHILLER/SOLVEQ codes). Dr. Yui asked about the precipitation behavior of SiO_2 minerals with respect to the long-term behavior prediction. Dr. Spycher answered that the principal mineral to precipitate was amorphous silica, from dissolution of rock-forming silicates (cristobalite, feldspars, and some quartz) followed by boiling (evaporative concentration).

Dr. Yui asked if DOE (Department of Energy, USA) was planning to extend the

TOUGHREACT code to include radionuclide transport. Dr. Spycher suggested that the code could easily include radionuclides using the thermodynamic database for radionuclides developed by LLNL. The code can also accommodate Kd's and surface complex models, providing input data are available for these models. Dr. Yui also asked about the possibility of including mechanical effects in the THC code. Dr. Spycher answered that the TH code, TOUGH2, has been coupled with the code, FLAC, and a coupled THM-THC code would be developed in the future.

Status of a Research Program for Numerical Experiments on the Coupled Thermo-Hydro-Mechanical and Chemical Processes in the Near-Field of a High-Level Radioactive Waste Repository

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ABSTRACT

In the near-field of a high-level radioactive waste (HLW) repository, the coupled thermo-hydro-mechanical and chemical (T-H-M-C) processes will occur, involving the interactive processes among radioactive decay heat from vitrified waste, infiltration of groundwater into buffer material, swelling pressure of buffer material due to saturation and chemical reaction between EBS material and porewater (Figure 1). Since observation periods by laboratory and in-situ experiments are very short and information by natural analogue studies is very limited, numerical experiments are the only available approach to predict the near-field long-term evolution.

The coupled T-H-M model has been already developed through laboratory, in-situ experiments and DECOVALEX project (Stephansson et al., 2001), and is to predict maximum temperature, resaturation time and mechanical stability during the resaturation of engineered barriers. To understand and assess the long-term performance of the near-field of a HLW repository, we have initiated a research for numerical experiments on the coupled T-H-M-C processes. The focal point of this research is to predict (1) near-field chemistry for overpack corrosion and radionuclide migration; and (2) near-field long-term integrity by chemical degradation.

To develop the coupled T-H-M-C model, we defined the interactions among each process and built the conceptual model for the coupled T-H-M-C processes (Figure 2). Although many kinds of chemical process are assumed in the near-field of a HLW repository, our current focal point is to take into account the interaction between minerals and porewater in buffer material

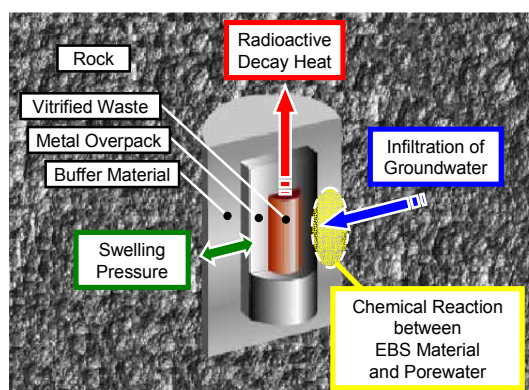


Figure 1. Schematic view of the geological disposal system and expected processes after emplacement of the engineered barriers

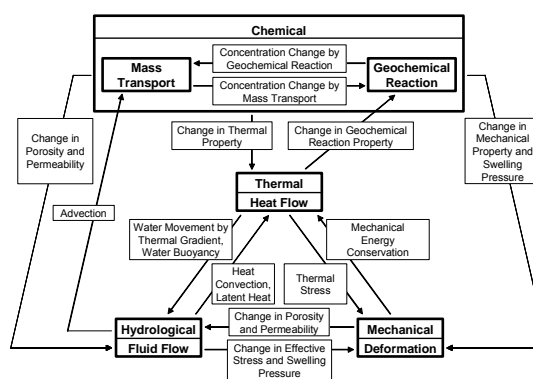


Figure 2. Conceptual model for the coupled T-H-M-C processes

and surrounding rock. Based on this conceptual model, we have developed the coupled T-H-M-C model and prototype code (Ito et al., 2003, Neyama et al., 2003).

The prototype code is based on the coupled T-H-M code “THAMES” (Chijimatsu et al., 1999), mass transport code “Dtransu-EL” (Nishigaki et al., 2001) and geochemical code “PHREEQE” (Parkhurst et al., 1980) which have been well verified and validated through benchmark tests and various experiments, and some of them are adopted in the second progress report on research and development for the geological disposal of HLW in Japan (H12 report; JNC, 2000).

Figure 3 and Figure 4 show the analytical results by the prototype code on the coupled processes in the near-field. The near-field geometry and heat output of vitrified waste are based on the H12 report. In this analysis, we assume that buffer material and backfill are composed of smectite, calcite and chalcedony; and that rock is composed of calcite and chalcedony.

The preliminary conclusion through demonstration analysis on the coupled processes in the near-field is that pH in buffer material highly depends on temperature. This is because solubility of calcite, which influences porewater pH, depends on temperature. In the near future, we will refine our model to take into account key processes on mass transport and geochemical reaction, e.g. gas transport, reaction of ionic exchange, surface complexation and kinetic reaction of dissolution/precipitation. And we also need to increase understanding on the processes in the compacted bentonite, e.g. liquid/vapor movement, and mass transport and geochemical reaction under unsaturated conditions.

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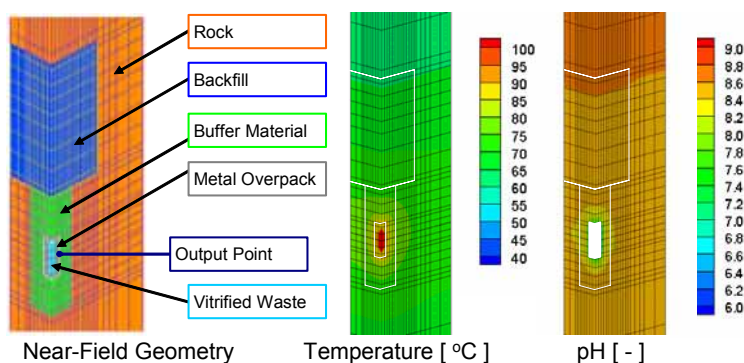


Figure 3. Near-field geometry for analysis and analytical results of temperature and pH distribution at 10 years after EBS emplacement

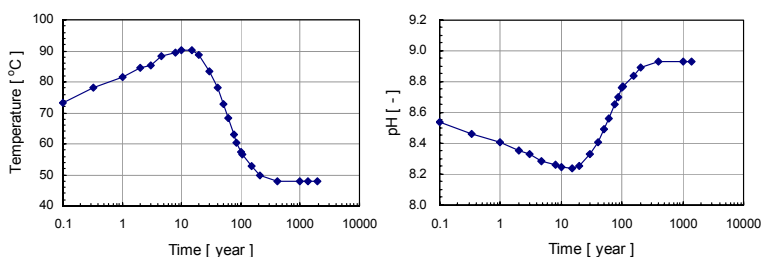


Figure 4. Time history of temperature and pH at output point (boundary between overpack and buffer material)

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MINUTE

Prior to the H12 report, JNC had developed the coupled THM model through laboratory, *in-situ* experiments and DECOVALEX project. This model is to predict maximum temperature in buffer material, resaturation time of engineered barriers, and mechanical stability during the resaturation of engineered barriers. Since the H12 report, we have initiated research on the coupled THMC processes in order to understand and assess the long-term performance of the near-field of a HLW repository. The focal point of this research is to predict 1) near-field chemistry for overpack corrosion and radionuclide migration; and 2) near-field long-term integrity by chemical degradation.

In the presentation, 1) a framework of research, 2) the development of the coupled THMC model, 3) a prototype code development on the coupled THMC processes, 4) a demonstration analysis of the developed code, 5) the laboratory experiment "COUPLE" on the coupled THMC processes, 6) encountered difficulties and 7) a conclusion are reported.

The preliminary conclusion through demonstration analysis on the coupled processes in the near-field is that the pH in the buffer material highly depends on temperature. This is because solubility of calcite, which influences porewater pH, depends on temperature. In the near future, JNC plans to refine our model to take into account key processes of mass transport and geochemical reaction, *e.g.*, gas transport, reaction of ion exchange, surface complexation and kinetic reaction of dissolution/precipitation of minerals. It is also necessary to increase the understanding of the processes in the compacted bentonite, *e.g.*, liquid/vapor movement, and mass transport and geochemical reaction under unsaturated conditions.

Main discussion points were saturation process in compacted bentonite and the methods of measuring pH and porewater chemistry. For the former issue, as discussed in the presentation by Dr. Patrik Sellin, an understanding of the saturation process in compacted bentonite is not enough and it is very difficult to clarify the saturated condition through observation. For the latter issue, Dr. Ochs commented on the difficulties of measuring the chemistry in compacted bentonite because of structural complexity, existence of different kinds of water *etc.* Dr. Ochs also asked about the reliability of the pH measurements using a glass ion-electrode. Mr. Ito answered that pH measurement by glass ion-electrode was reasonably successful in the small scale experiment but reliability of pH measurement in this experiment was not clear. Prof. Ohmoto suggested that the pH measurements using an ion sensitive field effect transistor in the experiment might be reasonable and the obtained result was real.

Development of Low Alkalinity Cement(HFSC) by Japan Nuclear Cycle Development Institute

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ABSTRACT

Construction of the repository requires the use of cement materials. It has however been indicated that normal cement materials may not only govern the chemical conditions of near field, but may alter of bentonite and surrounding host rocks. They may change the corrosion-behavior of the overpack, or may affect radionuclide migration behavior, leading to the difficulty in the safety analysis of the repository. In order to cope with these issues, JNC has developed a low alkalinity cement, HFSC(High Flyash contained Silica fume Cement). Constructability will be validated in the construction of underground facility at the HORONOBÉ test site.

Besides HFSC, several low alkalinity cements have been developed by different organizations, as shown in Table 1.

Table 1 Low alkalinity cements developed by different institutes

	HFSC	LAC-S	LHHPC	Low pH cement
Organization	JNC	CRIEPI	AECL	SKB, POSIVA
Country	Japan	Japan	Canada	Sweden
Type	Pozzolan mixture* ¹	Clinker design* ²	Pozzolan mixture* ¹	Pozzolan mixture* ¹
Base Cement	40wt%(OPC)	80wt%(LAC-C)	25wt%(OPC)	(OPC?)
Silica Fume	20wt%	20wt%	25wt%	used
Flyash	40wt%	—	—	—
Silica Flour	—	—	50wt%	Fine quartz
PH	< 11	< 11	< 10	?
Strength	> 40MPa(28day)	> 40MPa(28day)	> 70MPa(28day)	?

*1: Low pH values are obtained by mixing pozzolan(i.e., silica fume) with OPC

*2: The value of pH is lowered in the cement production stage, then adding silica fume

Low alkalinity cement may have to satisfy requirements such as low pH value, constructability, quality about compressive strength and durability, and economy. Low Alkalinity Cement has good durability itself, when used with steel (as rock bolts), but the durability has yet to be evaluated. JNC has measured the decrease in pH, and has conducted shotcreting test, compressive strength test, and corrosion test of re-bars to verify and satisfy the requirements.

From the results of the study carried out on HFSC to date, the use of Low Alkalinity Cement seems practical for underground repository, with a sufficient quality control for the amount of flyash used.

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corrosion-behavior of the overpack, and may affect radionuclide migration behavior, leading to the difficulty in the safety analysis of the repository. In order to cope with these issues, JNC has developed a low alkaline cement, HFSC (High Flyash contained Silica fume Cement). Constructability will be validated in the construction of the underground facility at the Horonobe test site.

Low alkaline cements have to satisfy requirements such as low pH value, constructability, quality about compressive strength and durability, and economy. Low alkaline cement has good durability itself, but when used with steel, the durability has not yet been evaluated. JNC has measured the decrease in pH and has conducted shotcreting tests, compressive strength tests, and corrosion tests on re-bar to verify and satisfy the requirements.

From the results of the study carried out on HFSC to date, the use of low alkaline cement seems practical for use in an underground repository, with sufficient quality control for the amount of flyash used.

Prof. Ohmoto pointed out the importance of measuring the silica content in the solution and explained the reason for the drop in pH in connection with hydration of silica species.

Dr. Ochs commented about the curing effects. The cement matrix may be different due to the cure rate of the concrete versus the length of the test. Most commercial cements have cure lengths that are 20-30 days. After only 3 days, pulverizing and adding it to water may promote additional hydration. It was recommended to analyze the samples used by XRD in order to identify the curing effects.

Dr. Svemar added that low alkaline cement was considered as grouting material in Sweden. Focal point is the same in that it is expected to reduce pH value.

Cement Degradation: Effects on Bentonite and Rock

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ABSTRACT

Introducing Portland cement into a repository setting sets up a situation where the adjacent materials (repository host rock and backfill) may be out of equilibrium with the groundwaters percolating through the site. Components leached from the concrete may destabilize minerals in surrounding rocks. Alternatively, components from the groundwaters may interact with, and degrade, the concrete. The residue from such interactions may, later, be leached from the concrete and initiate other reactions in adjacent rocks. All of these coupled processes make it difficult to predict whether the short-term benefits derived from using a widely available and trusted construction material will be offset by long-term adverse impacts on the repository.

One approach to answering such questions is to employ the wide variety of numerical models that already exist in the literature, or as commercially available computer codes. Numerical models range in complexity from simple empirical semiquantitative formulations, arising from the assembled wisdom of many years of civil engineering, to “state of the art” coupled transport –reaction path models. Several of these approaches are reviewed but emphasis will be on the results from the reaction path code called REACT. In a simulated shale environment the code suggests that Portland cement will react to a considerable extent in just a few decades (Fig.1). These studies also suggest that the adjacent rock composition is more important in determining the rate of reaction than is the chemistry of the leachate, coming from the concrete.

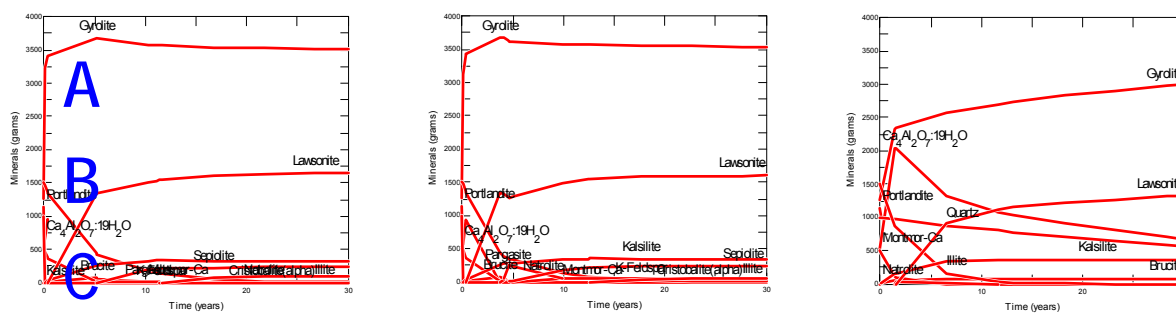


Fig. 1 Reactivity of model shale (1500 g Illite, 1000 g Silica, 500 g montmorillonite) with 3 kg simulated Portland cement. **A**: reactions using an aged pore fluid having a pH in the range 12.7 to 12.1. **B**: reactions in an early pore fluid with an initial pH of 13.4 and a final pH of 12.0. Cristobalite is the form of silica in both A and B. **C** represents what happens with an aged pore fluid when the form of silica is changed to Quartz.

Experimental studies represent the second approach to understanding the evolution of environment around a mass of Portland cement. Long-term tests (out to 5.5 years) were performed with mixtures of montmorillonite and $\text{Ca}(\text{OH})_2$. In samples that were just maintained at room temperature montmorillonite was still present after this time, though the presence of $\text{Ca}_4\text{Al}_2\text{O}_6\text{CO}_3 \cdot 11\text{H}_2\text{O}$ suggests some degradation of the montmorillonite. A second suite of samples experienced an early heat treatment (127 days at 90°C) that produced several zeolitic minerals not observed even after 5.5 years in the unheated samples. It also transformed the montmorillonite into a mixed-layer illite-smectite. The longevity of the montmorillonite (unheated experiments) and mixed-layer clay (heated experiments) strongly

suggests that the kinetic parameters currently available for modeling such systems theoretically may represent reactions that are much faster than really occur.

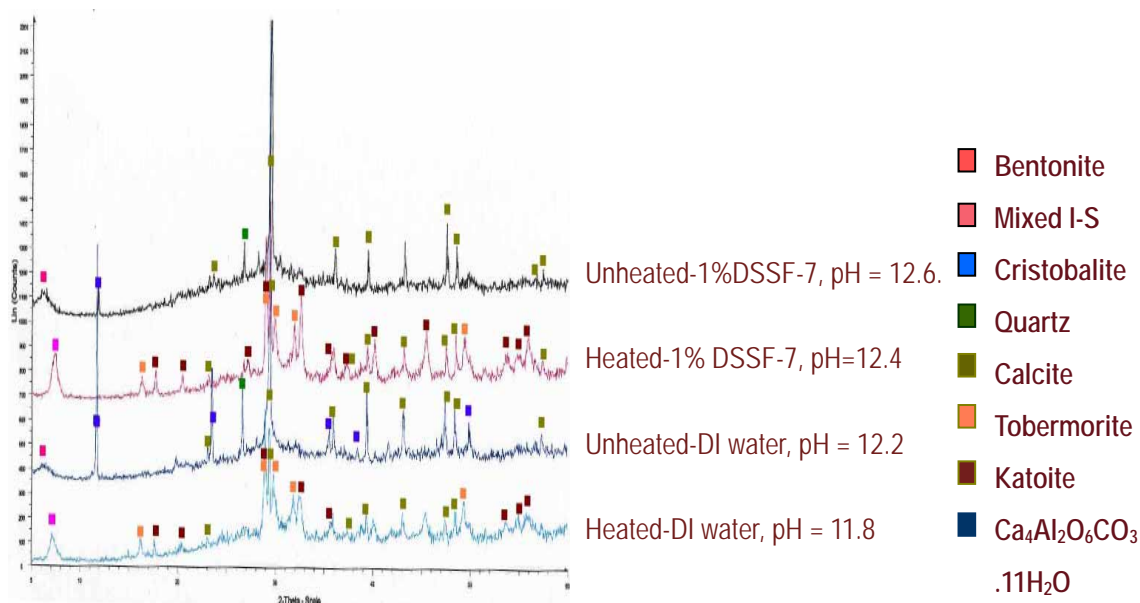


Fig. 2. X-ray diffraction pattern and mineralogy of montmorillonite plus $\text{Ca}(\text{OH})_2$. Samples were aged for 5.5 years. The pH values refer to measurements made after the systems had equilibrated for 5.5 years.

Analogue studies are the third approach to predicting the long-term fate of concrete in repository environments. Ancient cements have been thoroughly studied and suggest that rocks against a mass of Portland cement would only be altered at very slow rate, roughly a mm per thousand years at most. Another sort of analogue study was also initiated directed at understanding what happens on time scales of years to decades rather than millennia. In this study four different samples of discarded concrete were collected and crushed to various sieve sizes. Because of their location it is presumed that they had aged outside for several years, or possibly decades. Samples were characterized for mineralogy (X-ray diffraction) and texture (SEM) and then subjected to cycles of leaching (5-10 g concrete to 50 ml water). Even with just four samples a surprising range of pH values were noted in the leach water ranging from about 12.5 down to 10.5. Heating of some leaching experiments to 70°C revealed that increasing the temperature had a negligible effect on leach pH.

In combination, these studies emphasize the need for better reaction rate constants for use in theoretical models, the need for better coupled transport-reaction path models that will be more successful in representing the actual geometries of proposed repository designs (and hence mass balance relationships), and suggest that analogue studies dealing with intermediate-age processes could be quite fruitful.

Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under Contract DE-AC04-94AL85000

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Ordinary Portland cement "OPC" alters the adjacent materials (host rock and backfill) in the repository. The objective of this study is to predict the effects of OPC on the adjacent materials by combining several approaches such as numerical models, experimental studies and natural analogue studies.

Dr. Krumhansl showed the advantages and disadvantages for each approach. Numerical models have the advantage of providing long-term perspectives but there are disadvantages in the incomplete understanding of processes, incomplete databases, and numerous assumptions needed to set up models. Experimental studies provide “real world” constraints on models based on the actual chemical processes but can only provide short-term results, and there are size limitations. Natural analogue studies provide the data for intermediate to long-term “real-world” interactions but it is often impossible to know enough about the history to develop quantitative insights.

Empirical models and numerical models (reaction path models) using a commercially available computer code called REACT were presented. Empirical models are useful as screening tools to identify which processes will be important. Reaction path models are good for predicting how complex mixtures of materials will interact – such as when OPC is placed in contact with host rock and backfill. In a simulated shale environment (1500g illite, 1000g silica, 500g montmorillonite), the reaction path model suggests that OPC will react to a considerable extent in just a few decades. The results also suggest that the adjacent rock composition is more important in determining the rate of reaction than the chemistry of the leachate coming from the OPC.

Experimental studies were performed to understand the evolution of mineralogy around a mass of OPC. The results of long-term tests using mixtures of montmorillonite and $\text{Ca}(\text{OH})_2$ for 5.5 years show that montmorillonite was still present at room temperature, through the presence of $\text{Ca}_4\text{Al}_2\text{O}_6\text{CO}_3 \cdot \text{H}_2\text{O}$ indicated some montmorillonite degradation. On the other hand, when an similar mix was heated (127 days at 90°C) several zeolitic minerals and a mixed-layer illite-smectite were produced in a relatively short time. The longevity of the montmorillonite and mixed-layer illite-smectite suggests that the rates available for modeling may be much faster than really occur.

Natural analogue studies, using ancient cements, suggest that rocks against OPC are altered at a very slow rate, roughly a mm per thousand years at most. Results from an analogue leaching study using four randomly collected samples of aged concrete were also presented. These studies were carried out to ascertain how much variability in leach fluid pH one might expect after concretes that had been exposed to the weather for long periods of time (years or decades). Even with this limited number of samples a surprising range of leachate pH values were noted, with values ranging from 12.5 down to 10.5. As expected from the literature, the pH of the leachate does not drop much with multiple exchanges of water. This suggests that aging removes the primary high pH pore fluids rich in (K, Na) OH, and that after that the leach fluid pH is governed by the dissolution of phases that make up the bulk of the cement.

Discussion points in this presentation were a) modeling method and assumptions considered, b) applicability of accelerated experiment and c) availability of archaeological analogues.

Reaction path models have great utility in identifying differences in how various rocks will respond to contact with OPC. However, the models require several assumptions about thermodynamic data to be used, relative solid/solution ratios need to be considered in building the model, and phases that should not form in such environments need to eliminate from consideration. The selection of secondary minerals in the model calculation depends on the modeler’s expertise based on experimental and natural analogue data, but further knowledge about kinetic data in selecting assumptions is also required to investigate how rapidly changes happen. On the other hand, there are several models (*e.g.*, Atkinson, Berner *etc.*) to explain CSH gel behavior. The applicability of such models for long-term prediction should be checked against the experimental and natural analogues data.

With regards to the applicability of using accelerated experiments, there is considerable risk in using elevated temperatures to accelerate processes because the driving mechanism may change in comparison to room temperature. In the case of CSH gel, it may not be stable when the temperature is above 80°C.

The study of archaeological analogues is useful to enhance the confidence of long-term model prediction. Natural analogue studies for ancient concrete and the Maqarin site are well advanced but the use of more recent man-made analogues to address times ranging from decades to a few centuries has not been well investigated. Dr. Krumhansl suggests that the analogue site should be carefully prepared and 5 to 10 sites might be needed to gain confidence.

Coupling models and experimental studies, including natural analogues, may provide many useful constraints on how OPC actually interact with the host rock and backfill.

Stability of Bentonites and Formation of Secondary Minerals under Hyperalkaline Condition

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ABSTRACT

The envisaged extensive use of cement for encapsulation, backfilling, and grouting purposes in geological radioactive waste repositories can produce hyperalkaline pore fluids (pH 13.0 to 13.5) during its degradation. Potential migration of hyperalkaline pore fluids can degrade the surrounding bentonite buffer and host rocks effectively reducing their capacity to contain and retard migration of radionuclides. Formation and evolution of subsequent materials result as the migrating pore fluids eventually lower to moderately alkaline ranges after reaction with surrounding materials.

A key research issue in the performance assessment of radioactive waste disposal arose regarding the stability of smectite (a major component of bentonite) in bentonite-cement pore fluid interaction. Bentonites presumably lose their desirable properties as buffers resulting from the potential dissolution of smectites during the early stages of the interaction. An understanding of smectite dissolution behavior and rate under hyperalkaline conditions is imperative.

Mineralogical conversion during the interaction with high pH fluids, and its effect on swelling and sorption capacities have been roughly understood (for example; Johnston & Miller, 1984, Duerden, 1992, Savage et al., 1992, Eberl et al., 1993, Bauer & Berger, 1998, Amaya et al., 1999 and Sato, 2001). Previous studies mostly focus on mineral conversion under high pH and high temperature conditions, and only a few conducted experiments under varying pHs and at temperatures similar to repository conditions. Although the data obtained from these studies are reliable, it is difficult to compare results of various experiments and *a priori* discussion on the effects of pH on the dissolution of smectite. The primary reason is attributed to differences in smectite purity used in the experiments, some of which contains other minerals (i.e. cristobalite, quartz, calcite, etc.). Cama et al. (2000) used an illite/smectite interstratified mineral (85-90% smectite), although their experiments is considered to be the most excellent and systematic among the previous studies. Secondly, the dissolution experiments utilized different systems (i.e. flow-through (open) or batch (closed) systems). In batch systems used by most studies, the degree of saturation changes through time (i.e. deviation from equilibrium) wherein smectite dissolution rates do not attain a constant rate (Oelkers et al., 2001).

Stirred flow-through systems under neutral to highly alkaline conditions were performed to determine more reliable smectite dissolution rates, and to elucidate the effects of pH. An understanding of the mechanisms of smectite dissolution was achieved with the aid of Atomic Force Microscopy (AFM) and Attenuated Total Reflection Infrared Spectroscopy (ATR-IR). The experiments were conducted for mixed NaOH-NaCl and KOH-KCl aqueous solutions (I = 0.3 M). Purified smectite (Kunipia-P® from Kunimine Industry Co. Ltd.) was reacted from pH 8 to pH 13, at different temperatures (T = 30, 50, 70°C).

Dissolution rates were calculated from steady-state Si and Al concentrations. Preparation of stock input solutions and output solutions sampling were done inside a glove box in a N₂-gas environment. Smectite dissolution mechanisms were observed *in situ* by AFM fitted with a fluid cell and ATR-IR.

Smectite dissolution rates increased with increasing pH (pH = 8 to 13). The effect of pH on the dissolution rate is clearly shown in Figure 1. Furthermore, interlayer species present in smectites have no effect on smectite dissolution rates and can be shown by comparison of the dissolution rates between the NaOH-NaCl and KOH-KCl systems (Fig. 1). Rate laws are calculated by plotting the dissolution rates against the pH of the output solution. At 50°C in NaOH-NaCl solution, the following equation was obtained from Si concentration:

$$\text{Rate (mol m}^{-2} \text{ s}^{-1}) = 10^{-14.11} a_{\text{H}^+}^{-0.25} \text{ (in NaOH solution).}$$

The effects of pH condition on smectite dissolution rate varies at different temperatures. Furthermore, activation energy of the dissolution reaction is also different. The activation energy ranges from 27 kJmol⁻¹ at lower pH to 62 kJmol⁻¹ at higher pH. The relationship between activation energy and pH is represented by the equation:

$$E_{\text{exp}} = 6.04\text{pH} - 16.51 \quad (> \text{pH } 8)$$

Variation in activation energy with pH at elevated temperatures increasingly influence dissolution rates which is also observed for other minerals such as kaolinite in alkaline conditions.

AFM images taken during the dissolution experiments reveal different dissolution behaviors of smectite under acidic and alkaline conditions. Under acidic condition, individual particles exclusively dissolve on their edge surfaces. No basal surface dissolution occurs under acidic conditions as etch pits did not develop. Under alkaline condition, individual particles dissolve both on the edge and basal surfaces. Etch pits formed on basal surfaces which links with other etch pits as the dissolution reaction progresses.

In the ENTRY workshop, we intend to introduce our natural analogue study of secondary mineral formation and associated fracture fillings around hyperalkaline thermal springs in the Oman ophiolite.

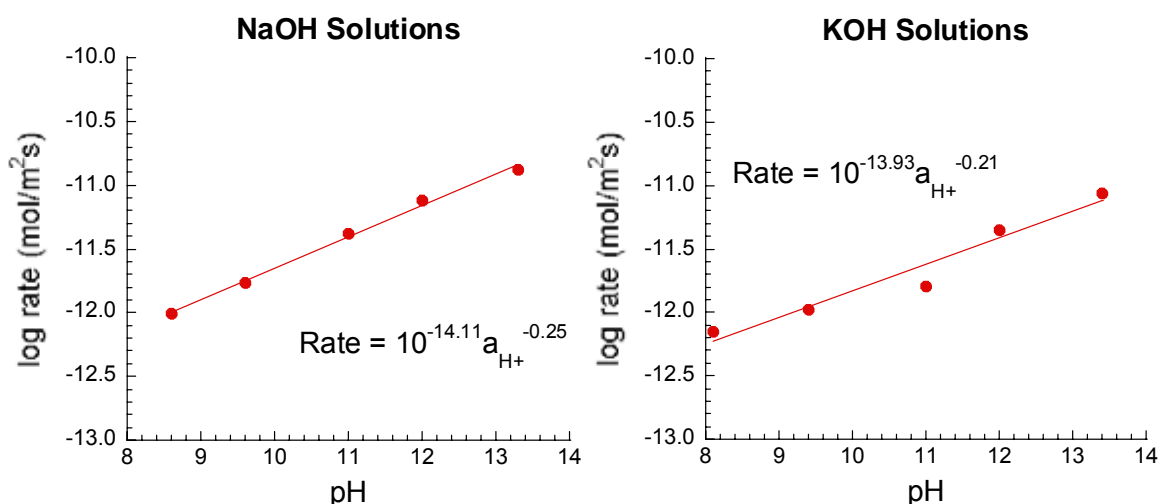


Figure 1. Relationship between logarithm of the dissolution rates and the pH of the solution in NaOH-NaCl (left) and KOH-KCl (right) systems.

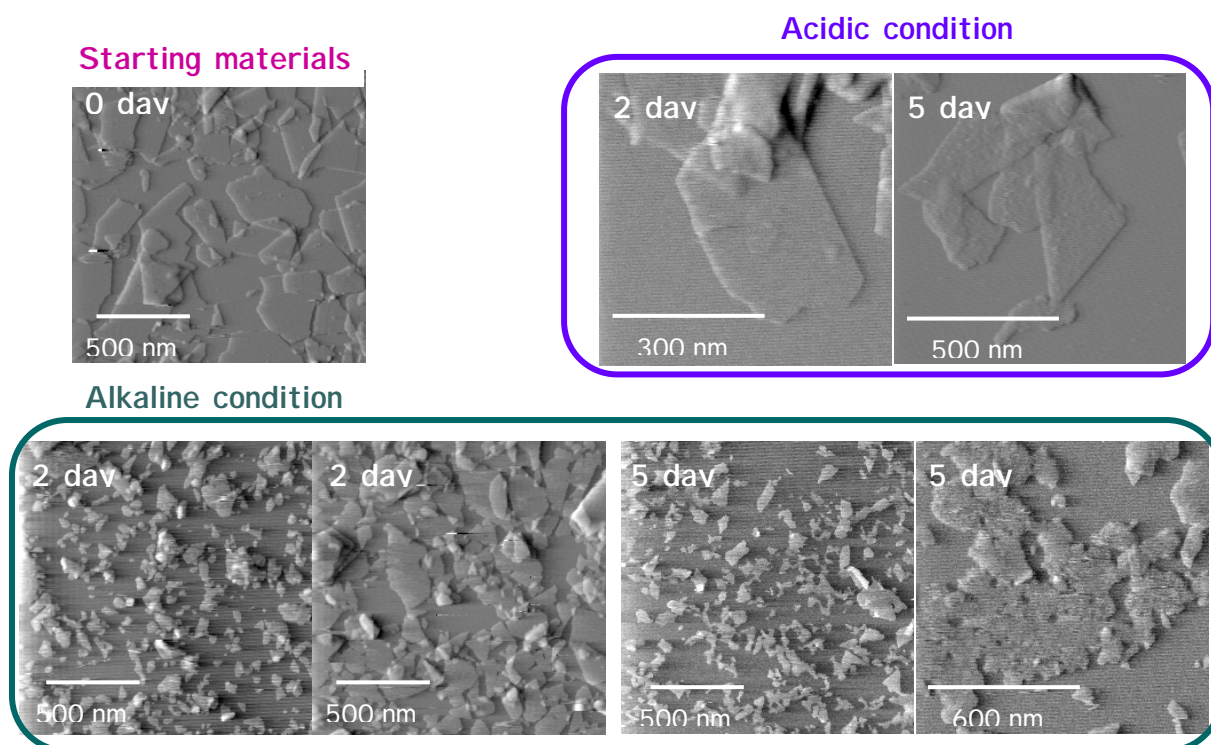


Figure 2. AFM images of starting smectite before and after reactions under acidic (pH 1.0) and alkaline (pH 13.3) conditions.

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Hyperalkaline fluids can degrade the host rocks and bentonite buffer effectively reducing their capacity to retard the migration of radionuclides. Thus, the stability of smectite (a major component of bentonite) is a key issue for the performance assessment of radioactive waste disposal. Dr. Sato presented the results of experimental studies about smectite dissolution rate under hyperalkaline conditions and a natural analogue study of secondary mineral formation around a hyperalkaline spring in Oman.

A stirred flow-through system was used to determine the reliable smectite dissolution rates. The experiments were carried out using mixed NaOH-NaCl and KOH-KCl solution ($I=0.3M$). Purified smectite (Kunipia-P) was reacted at pH 8 to pH 13 at different temperatures ($T=30, 50, 70^{\circ}C$). Smectite dissolution mechanisms were revealed by the microscopic technique using AFM (Atomic Force Microscopy). Dissolution rates of smectite were calculated using steady-state concentrations of Si and Al. The rate laws were determined by fitting the dissolution rates against pH for each temperature as follows: Rate ($\text{mol}/\text{m}^2\text{s}$) = $10^{-13.79} a_{H^+}^{-0.27}$ ($T=70^{\circ}C$), $10^{-14.11} a_{H^+}^{-0.25}$ ($T=50^{\circ}C$) and $10^{-13.65} a_{H^+}^{-0.15}$ ($T=30^{\circ}C$). The activation energy increases from 27 kJ/mol to 62 kJ/mol with pH. The rate laws were obtained in the water dominated conditions, but the mineral (*i.e.*, smectite) dominated in the compacted bentonite. It should be noted that several effects (anionic exclusion, effective surface area, physico-chemical properties of water and cementation by secondary minerals) might be considered when the rate law data are applied to the system of compacted bentonite. On the other hand, AFM observations showed the difference of smectite dissolution behaviors under acidic and alkaline conditions. Smectite particles mainly dissolve on the edge surfaces under acidic condition, but the particles dissolve both on the edge and basal surface under alkaline condition.

The results of the field investigation in Oman show that the fractures in ophiolite are filled with several minerals (calcite, aragonite, hydromagnesite and other small amount of minerals not detected by XRD) as the secondary alteration minerals caused by natural hyperalkaline fluids.

Discussion points in this presentation were a) an experimental system to determine the smectite dissolution rate, b) the differences of dissolution rate by experimental conditions and c) a new method to determine the dissolution rate.

The dissolution rate of smectite strongly depends on the experimental system (*i.e.*, flow-through or batch systems). In the case of batch system, the smectite dissolution rate does not reach a constant value because the saturation degree changes during the experiment. A flow-through system is recommended to determine a reliable dissolution rate of smectite.

The residence time of solutions in the reactors was discussed to clarify whether the dissolution rates obtained could be categorized as the initial dissolution rate. Prof. Ohmoto suggests that 10 hrs as residence time might be too long to determine the initial dissolution rate (R_{INT}) and the dissolution rate obtained should be categorized as the long-term dissolution rate (R_{LT}).

A new method to determine the dissolution rate using AFM observation was presented by Dr. Sato. This method can calculate the dissolution rate considering the volume changes of the smectite particle with time. Dr. Sato answered that the dissolution rate calculated by AFM observation was quite consistent with the rate calculated by Si and Al concentrations in the solution.

Understanding and Thermodynamic Modeling of Radionuclide Sorption on Bentonite and Rocks – Recent Progress and Challenges

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ABSTRACT

A central issue to the safe disposal of nuclear waste is the prevention or sufficient retardation of radionuclide migration to the biosphere. Almost invariably, 2 parameters are used in performance assessments of nuclear waste repositories to quantify the mobility of radionuclides along this migration path:

- The maximum solubility of a particular radionuclide in the relevant (homogeneous) solutions
- The partitioning of dissolved radionuclides between the solution and solids that make up the engineered and natural barriers, typically quantified by equilibrium distribution coefficients (K_d):

$$K_d [\text{m}^3/\text{kg}] = \frac{\text{stoichiometric sum of surface species of element X} [\text{mol/kg}]}{\text{stoichiometric sum of solution species of element X} [\text{mol/m}^3]}$$

While K_d values for a given radionuclide and a given set of conditions can be determined in batch experiments with a fairly high level of certainty, it is realized that K_d values are only valid for the specified conditions. However, K_d values to be used in performance assessment typically have to be derived for situations for which only few, if any, direct K_d measurements are available. This concerns a range of materials that are difficult to access experimentally and that represent complex sorbents, e.g. compacted bentonite, or fracture infill. Moreover, most performance assessments have to deal with alternative or "what-if" scenarios that require the derivation of situation-specific K_d values.

To derive such values in a reliable and transparent fashion, and to handle parameter uncertainty, a good understanding of the governing processes for radionuclide sorption is necessary. It has been pointed out by [1] that uncertainties in K_d as a function of variable geochemical conditions can significantly affect the apparent performance of a repository. Using selected examples, it will be illustrated in this contribution how recent advances in the investigation of sorption onto complex materials can facilitate the derivation of K_d values as a function of conditions for PA, and where, to the author's belief, lie the greatest future challenges.

For single, well-defined sorbents, such as metal oxides and pure clay minerals, a range of very successful thermodynamic sorption models (TSMs) has been developed to date [2-4]. These models, together with the underlying datasets and additional spectroscopic information, greatly aid in understanding and quantifying the effect of various geochemical parameters (pH, $p\text{CO}_2$...) on radionuclide sorption; they provide a vastly better tool for handling the relation between K_d and overall geochemistry than the traditional K_d and isotherm models.

Today, the main challenge is the transfer of this knowledge to PA purposes. This will require, in terms of conceptual understanding as well as actual modeling, to apply the information for single minerals to more complex sorbents, such as whole clays and rocks. This can be done in two different ways (see e.g. [5]):

- A K_d for a complex material can be derived based on the additive contribution of the individual minerals (bottom-up or component-additivity, CA, approach), or
- a given complex material can be treated more empirically as a black-box, with new information based on direct, material-specific experimental evidence (top-down or generalized-composite, GC, approach).

These different approaches have been a matter of debate during the last years. While for very complex sorbents the GC approach may well be the only realistic possibility, it will be argued that the level of complexity observed for many sorbents relevant for nuclear waste disposal, and in particular for bentonite, allows the application of CA-TSMs. It will further be illustrated that these approaches offer greater process understanding and, thus, greater predictive capability.

As a matter of fact, much of the apparent complexity of bentonite can be attributed to the porewater chemistry (e.g. [6]), whereas the actual sorption processes can be treated as for single clay minerals. Similarly, many rock systems appear to be dominated by only a few mineral components, allowing the application of CA approaches [7]. Overall, apparent discrepancies can in many cases be alleviated by paying appropriate attention to geo- or porewater chemistry. In no small part, progress in understanding sorption is due to this awareness. This holds also for linking sorption with diffusion, which is ultimately needed to obtain a consistent picture of radionuclide migration (e.g. [8]).

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MINUTE

The K_d value is one of the key parameters used in performance assessment of nuclear waste repositories to quantify radionuclide migration behavior in the bentonite buffer or rock. However, K_d values are highly conditional, and it is difficult to obtain K_d under repository relevant conditions from laboratory experiments. Further uncertainties in K_d values for PA are caused by chemical variability of groundwater and other conditions. Modeling of sorption behavior through thermodynamic sorption models (TSMs) as an important tool for K_d selection has been the subject of the OECD/NEA Sorption Project, and some selected results based on the were discussed in the presentation.

The focal points of this presentation were to show a) how to use the thermodynamic sorption models (TSMs) for single minerals, *e.g.*, pure clay minerals, and b) how to model K_d for complex sorbents, such as natural rock, fracture infill or organic containing soil. For a), surface complexation and ion exchange models are used. For b), adequate component models for single minerals can be used (Component Additivity (CA) model) or a Generalised Composite (GC) model is adopted. Based on the CA model, K_d is calculated by summing up the contribution to K_d for each single material constituting the complex sorbent. In the case that a substrate cannot be well characterized, K_d is calculated based on the GC model, in which the sorption parameters are derived from mathematical fitting of experimental data under the assumption of generalized sites.

In spite of the success of these models, complexity of sorption still remains even in the case of simple minerals. , Often, this is due to a complex porewater chemistry. As the porewater chemistry strongly affects the sorption behavior of radionuclides, reliable experimental results for detailed THMC model prediction and/or highly alkaline solution model are extremely important.

We don't have to take the effect of precipitation or co-precipitation into account in this discussion because only data in the area in which those effects are negligible is used for comparison with experimental data (e.g., cement systems are not treated in this discussion).

Though some useful, excellent datasets have been developed and opened, for example by PSI, none of them is so complete as to cover a wide range of minerals and elements.

It is possible that the disagreement between K_d acquired by batch sorption and in intact condition is mainly caused by the difference of porewater composition. If the batch experiments are carried out in the same solution as porewater, it is expected that the K_d values will be of the same order of magnitude as those obtained in the intact condition.

By far the most significant flaw of available studies is the lack of systematic or sufficient parameter variations, which are needed to develop an appropriate (robust) model. The progress of thermodynamic database and porewater chemistry is also important.

Aqueous geochemical modeling codes, for example PHREEQC, are components of a coupling THMC code. That is why the progress of TSMs, and the development of the underlying experimental data, is strongly important for the long term prediction of radionuclide migration.

Discussion on the State-of-the-Art for Long-Term Prediction

All Participants

MINUTE

According to a request from the previous evening by the Session 1 manager, Prof. Ohmoto presented his opinion about the stability of bentonite under repository condition. He explained the difference between apparent dissolution (*i.e.*, including the effect of precipitation) and true dissolution again. Also, he pointed out the buffer capacity of bentonite to neutralize the effect of high pH solution caused by the dissolution of cement materials. At that time, solid (bentonite) to solid (cement materials) ratio (in other words, *mass balance*) is a key factor to estimate the longevity of bentonite in the repository.

In relation to Prof. Ohmoto's presentation, Dr. Yamaguchi showed the experimental results of dissolution behavior in compacted bentonite under high pH condition. The results indicate that smectite dissolution in compacted/closed systems is slower than that in batch/open systems because of Si and Al saturation, and precipitation.

At present, models and data to estimate the longevity of bentonite are not enough for a reliable prediction of long-term behavior. Further strong linkage among laboratory experiments, field studies, and modeling are needed and should be continued.

There were discussions about difficulties without cement case. Key discussion was about saturation in compacted bentonite and Dr. Dixon suggested that critical time scale might be length of pre-saturation. Prof. Ohmoto commented that it would be beneficial to have a good understanding of how groundwater flows through the bentonite.

Natural analogues are not well-defined controlled systems, but they can provide useful information quantitatively under certain circumstances. Natural analogues and archaeological analogues can be good tools for convincing the public as to the veracity of the science. An URL (Underground Research Laboratory) is also a very good PR tool, because it demonstrates experience in the environment.

HMC Model Development for TRU Waste Repository

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MINUTE

Mr. Mihara presented the JNC's HMC model for the TRU waste disposal. First, he reported the development of a detailed 1-D, full kinetic chemical/transport coupling model for the multi-component system (cementitious material and bentonite) and its preliminary results. A Cam-clay mechanical model which could describe the swelling of bentonite influenced by cementitious material was also developed. Second, he showed an example of analysis results of a prototype HMC model which consisted of hydrological, mechanical and simplified chemical modules.

It was pointed out that 1-D chemical/transport coupling analyses suggested some inhabitation of montmorillonite dissolution by pH buffering and the sacrificial dissolution of the additive silica sand. The participants recognized the kinetics of montomillonite dissolution is more important based on the comparison of the results of kinetic model analyses with those of equilibrium model analyses. The latest information of its kinetics will be reflected in future models and sensitivity analyses will be conducted by JNC for identifying the important parameters. The importance of both verification of the analytical assumptions and of cross-checking with other similar codes was discussed. Mr. Mihara plans to conduct the comparison of the JNC chemical model with other models (*e.g.*, PRECIP). A clogging indicated by 1-D chemical/transport model due to the precipitation of calcite in cement zone was also commented upon. The necessity of a 2-D model analysis was recommended and Mr. Mihara answered that their fully coupled HC model will be extended to 2D in this fiscal year.

The importance of the surface area of bentonite applied in the analysis was discussed and it was recognized that there is a big difference between a theoretical surface area including interlayer (about 800m²/g) and a grain surface (not including interlayer) measured by BET (about 30m²/g).

Dr. Yui inquired about the role of the coupling model in the next PA reporting. Mr. Shiotsuki suggested that the model will be reflected in the next PA reporting, but not directly incorporated, because the hydrology of the near field was identified to be one of the most important factors in PA results of the TRU waste disposal.

Wrap Up
- Introduction of summaries of the session I and of II and Discussions -

All Participants

MINUTE

Summary of Session 1

Session 1 manager, Dr. Yui, in an overview, summarized the presentations and discussions held in Session 1 over the course of 3 days. First, he gave a brief summary of each presentation that was given in Session 1.

AECL in Canada has carried out valuable *in-situ* experiments in Whiteshell URL. A large database for demonstration of technology and THM numerical models has been developed.

The on-going prototype repository project at Äspö in Sweden by SKB provides a good example for demonstration of technology, numerical models development of THM and C, and clarification of difficulties in understanding (*e.g.*, micro structure of clay, creep *etc.*).

Numerical simulation of THM by LLNL in the USA provides a design of long-term monitoring programs that take into account complex effects in the repository and shows the possibility of fully integrated/scalable simulations.

Numerical modeling of THM by LBNL in USA provides an application for the Yucca Mountain site through validation and long-term prediction analyses of repository evolution. Models used in the analyses are validated by laboratory experiments.

Numerical experiments of THMC by JNC in Japan were initiated after the H12 report and show the demonstration analysis to confirm H12 analysis. A new COUPLE experiment started in ENTRY facility at Tokai Works to test an applicability of prototype THMC code developed by JNC.

Development of low alkaline cement by JNC shows the comparison in performance of low alkaline cements in the world and practicality of HFSC for URL construction.

Modeling, laboratory experiments, and natural analogue studies for concrete degradation and bentonite alteration performed by SNL, in USA, shows the importance of coupling with models and experimental studies including natural analogues and the necessity for a better understanding of concrete degradation phenomena using archaeological analogues (*e.g.*, recent man-made concrete materials).

Bentonite alteration experiments under hyper-alkaline conditions by Kanazawa University in Japan provide a valuable experimental basis of understanding for smectite dissolution. Also, natural analogue studies of Oman ophiolite show important information about secondary mineral formation under hyper-alkaline conditions.

Radionuclide migration mechanisms presented by BMG in Switzerland shows how to use the thermodynamic sorption models and how to model K_d for complex sorbents. Ion exchange (IE) and surface complexation (SC) models are available for the use in thermodynamic sorption models. An understanding of sorption from simple to complex minerals is possible through the use of the component additivity (CA) model and the generalized composite (GC) model.

HMC model development by JNC for TRU waste disposal in Japan shows a chemical/transport coupling model for bentonite-cement interaction and an adoption of recent chemical/mechanical (creep) models. Verification/validation studies, sensitivity analysis for identifying the important parameters, and confirmation of surface area of bentonite are needed for further improvement of models.

Next, Dr. Yui presented the following results of the discussion in Session 1.

Discussion point 1: What is the state-of-the-art for long-term prediction of near-field ?

A big issue for long-term prediction of near-field is the cement effect. Kinetic interpretation of smectite dissolution under high pH condition is still debatable and the necessity of estimation for smectite dissolution rates in compacted bentonite is recognized because the compaction effect on smectite dissolution rates is significant. Also, the balance on consumption of alkaline by present, non-smectite materials such as other minerals/backfills/rocks suggests that alkaline perturbation may not significantly affect the performance of the engineered barriers. Knowledge about secondary minerals under hyper-alkaline condition is not enough and further investigation should be continued. A greater understanding of the saturation processes of bentonite needs to be gained especially from the view points of chemistry and mechanics (*e.g.*, creep), and to be linked with long-term behavior. A lack of a basic database, such as a kinetic database of mineral dissolution under high pH conditions, is recognized. Not only THC coupling model but also THM coupling model may be needed for the further research in Yucca Mountain project. Numerical simulation/experiment and quantitative interpretation of natural analogue should be performed in a step-by-step approach. Engineering technology (*e.g.*, design and construction of repository *etc.*) should be strongly linked with the long-term prediction of the near-field.

Discussion point 2: What are the limitations of laboratory and *in-situ* experiments and natural analogues? What are their roles? How to concert them?

A basic procedure like a step-by-step approach (*e.g.*, small scale experiments in laboratory→large scale experiments in laboratory→*in-situ* experiments in URL→experiments in real repository) is very important for a better phenomenological understanding and demonstration of repository. The limitations of experiments in URL are strongly related to the length of time for experiments (maximum time might be orders of decade), a limited use of radioactive elements, and a poor understanding of geochemical phenomena. More relevant natural analogues (*e.g.*, archaeological analogues) should be investigated quantitatively. The importance of communication between modelers and experimenters is recognized, because it is through communication that the individual role of each expertise and field of study is defined and established. It is also important to understand the initial condition of phenomena determined through short-term controlled laboratory experiments. Finally, it is necessary to have a good conductor who can concert (or manage) the valuable results of modeling, experiments, and natural analogues while also properly considering various (and sometimes contradictory) opinions from different fields of experts.

Discussion point 3: What is the relevance of numerical experiments?

The role of numerical experiments in the performance assessment (worst case and/or conservative case) and in the realistic prediction of repository evolution needs to be identified. Also, continuously refining models based on discussions by various fields of experts is necessary. A step-by-step approach is important for refining the models. Verification and validation should be carried out to determine the relevance of numerical experiments. We also have to recognize that there is a limitation of computer capability for numerical experiments.

Discussion point 4: How to link among different areas/experts?

This workshop is a very good chance for people to communicate with experts from different areas of study. Also, coffee breaks during the workshop provide participants to informally discuss areas of mutual interest. These informal chats can lead to greater understanding of technical issues in other fields of interest as well as provide contacts for future communications. It is necessary for various fields of experts to participate in discussions during the planning and design phases of THMC coupling experiments.

Discussion point 5: How to concert internationally for real prediction?

Science progresses continuously. International concert and cooperation are very valuable to obtain the latest information in the world. EC projects (e.g., FEBEX, PRP, NET, EXEL, EDSRED, NF-PRO) are very important for better understanding of coupling phenomena and increasing reliability of models.

Discussion point 6: Reliability of mechanistic databases (kinetics, thermodynamics *etc.*)

Lack of reliable databases, especially kinetic data for mineral dissolution rates under high pH condition, is recognized and further laboratory experiments should be carried out.

Discussion point 7: Scenario analysis to be replaced by mechanistic modeling?

At present, it is dangerous for mechanistic modeling to completely replace scenario analysis. Mechanistic modeling should be used for supporting scenario analysis.

Finally, Dr. Yui introduced the key words from the participants to increase confidence for long-term behavior prediction as follows (the number in parentheses is the number of people giving that response). All workshop participants and supporting staff were given an opportunity to respond.

- Understanding (5), communication (4), coupling (3), real/reliable database (3), testing (2), sensitivity analysis (2), coordination (2), consistency, uncertainty, uncertainty and similarity in NA, relevance, lack, kinetics and mechanism, low alkaline cement, assumptions and verification, applicability, validation, top-down and bottom-up, communication with other fields/researchers, promotion by JNC, stable funding.

Session 2

Objective/Goals of ISI and desired output from ISI

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ANDRA

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MINUTE

Presented and Session lead by Tom Doe

TD pointed out that there are at least two different objectives for conducting ISI. One is to rank the sites among a group of candidate sites, and the other is to assess the site suitability. The former can only compare the sites, but the danger is that ranking sites without suitability criteria could lead to choosing an unsuitable site.

TD classified events into “anticipated event” and “unanticipated event.” An anticipated event is a critical condition that is known to be possible but is not necessarily expected. For example, the French program does not expect conducting fractures in its argillite, but it will do drilling and testing to check the possibilities. Finding a conducting fracture would be an anticipated event (not expected but known to be possible). An unanticipated event is a critical condition not foreseen at all in the geologic conceptual model or included in the Performance Assessment (PA). An example of an unanticipated event is the compartmentalization of the TASK 3-2 area of the Kamaishi Mine. This is actually a favorable condition where fracture networks are mutually isolated. This unanticipated event appeared because there were good monitoring data, and data review revealed the condition. The lesson is that programs must be designed for both anticipated and unanticipated events. Anticipated events are studied using investigations specifically to test their existence. Unanticipated events are discovered by careful analysis of monitoring and other experimental data for consistency with conceptual models of site properties and behaviors.

Questions and answers

SM and KK asked for clarification of unanticipated events and TD answered that unanticipated events could be a FEP that was screened out incorrectly or was never on the FEP list, and also can be said as a surprise. TD cited examples such as testing for conductive fractures in French argillite, even though they are not expected, and for an unanticipated event the extreme compartmentalization of fracture networks in the Kamaishi mine. TD stressed the need for testing, monitoring and characterizing in great detail and paying attention to inconsistencies in the data.

BF agreed with the importance of a broad understanding of the site with reference to diffusion as the main process in PA of the Opalinus clay site and broad understanding of the site could be achieved with core sampling, water sampling by squeezing and isotope analysis allowed to show the process is valid.

Feasibility of ranking and suitability was discussed. AS explained that SKB developed the suitability indicators and criteria, but these were not developed for ranking but to confirm that

all of the requirements are fulfilled. This is to have certain minimum suitability criteria, which are indicators based on a PA. AH pointed out the difficulty for a program to look at the “best site,” since the uncertainties would be bigger than differences between the sites even after characterization with all possible geophysical methods and boreholes. AH also pointed out the importance of societal issues so that levels of the decision or what should be decided at which stage should be very carefully thought over. This is the key to go on with the suitability assessment and criteria at certain predefined steps. BF also pointed out the importance of social and economic factors, since Wellenberg was cancelled by a social factor.

AH explained the necessity of studying a group of candidate sites to show that the site condition is at least up to the same level as the general bedrock, since there are bad portions in the bedrock and one should be careful not to select a site that contains one of these bad areas.

The Yucca Mountain (YM) chlorine-36 event was discussed and it was recognized as an unanticipated event. In 1987, YM was selected as the sole site in the U.S., and the consensus of science was that significant amounts of unsaturated fracture flow was impossible. However, new information shows that if there exist wide-open fractures, film flow goes very fast.

What level of details do you aim at for modeling (conceptual, numerical, PA) as the result of ISI

LEVEL OF DETAILS

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ABSTRACT

The critical issues that are necessary to be addressed during ISI can be considered at different scales. The ISI studies should address all these scales. The regional geologic setting gives the starting point. A site should be not too close to major tectonic features that may be of risk for the repository. Such features include, for example, major crushed zones usually seen as lineaments of large extent. Analyzing the regional setting should result in an understanding of larger scale faults and occurrence of rock types as well as frequency of smaller scale fracture zones.

In the site scale the system of smaller scale fracture zones should be understood as a basis to assess if there is potential to locate the repository at that site. Questions like what limits and bounds rock volumes that could host the repository (or parts of it) have to be answered.

In the repository scale (tunnel and shaft system and auxiliary rooms) the number of minor fracture zones or other geological features cross-cutting the repository as a whole should be assessed. The properties of the main rock mass have to be known for construction and preliminary safety assessment purposes. These include the fracturing and hydraulic, rock mechanical, thermal, and geochemical properties. The rock properties are usually very heterogeneous but larger scale averages may be relevant instead of just local values.

The most detailed scale and level is the rock around the canister positions. Modeling should aim at rather detailed level and heterogeneities play a big role. It is, however, most difficult to acquire all needed data. Existing data should be used as efficiently as possible and uncertainties should be dealt with sensitivity studies. More data for this scale and detailed modeling can be gathered in the underground investigation phase.

MINUTE

Session lead by Anders Ström

Presented by Aimo Hautojärvi

AH considers understanding of the site is very important during ISI. In crystalline rock, fractures (fault) in different scales occur as self similar (fractal). POSIVA uses the block approach which defines the average rock by discriminating large features, since the property of the large features significantly differs from average rock. POSIVA classifies features into 1st order to 4th order.

AH presented critical issues at each scale as follows;

- Regional scale : lineaments and the 1st and 2nd class structures should be far away from the repository from the view point of 1) more likely to cause earthquakes, 2) possible to cause secondary movement. These structures could form hydraulic boundary conditions. These features can be somewhat uncertain but this needs to be allowed.

- Site scale: site scale rock volume should have good quality for the repository. With limited number of boreholes in ISI, the goal should be rather modest and critical issues will be structure and geology and we should not pay too much attention to small scale structures. The 2nd class structures will be the main conductors and form the boundary condition for rock mechanics. Small scale structure (single fracture) in block scale should have adequate properties to repository.

There are several ways of modeling, but AH pointed out that the data will not be sufficient for the DFN or channel network modeling and these models need to use generic data in a way not contradicting with site data. The whole picture of flow regime and boundary conditions are more important at this stage. Other important features and processes for the overall picture are 1) geochemical condition coupled with hydrology including bacteria, so that the origin of the groundwater chemistry can be explained and the future chemical evolution can be predicted, 2) the rock mechanics to understand whether the repository can be constructed, 3) thermal properties which control the volume necessary for the repository, and 4) the discharge area for the biosphere assessment needs to be addressed in general way, although understanding of exact location can be difficult at this stage.

The critical issues to determine the suitability of the site are;

- No adverse features (geological, hydrological, geochemical, rock mechanical),
- Enough area for repository (desirable to have more area than required to avoid bad portions).

The safety assessment at the end of ISI should integrate all scales and disciplines, but we should be rather modest at this stage. Even having separate modeling of hydrology, groundwater chemistry, and rock mechanics can be sufficient to judge whether we should continue the site investigation.

AH explained the limitation of DFN modeling at this stage by referring to the POSIVA flow log. The flow log has 10cm resolution and we can obtain detailed data, but these are still only 1D data and we can't drill many boreholes because it is not just time consuming and expensive but also damages the site. In later stage, we can obtain detailed data in the underground and this will be the time to use DFN model. But, we could still judge the quality of the host rock with the DFN model by extrapolating 1D information into 3D space, unless we have strong bias by drilling orientation against fracture orientation.

Questions and answers

MU questioned whether POSIVA conducted the sensitivity analysis of DFN model on fracture size, which is the most uncertain parameter. AH replied that single features or minor fracture zones have high transmissivities but these occur rather in a small percentage of the site, such as 1-2%, and there is very little to be analyzed and one has to have a strategy to avoid those. MU further questioned the avoidance criteria. AH answered that it depends on the flow rates and properties. These features exist with spacing of several tens, or even sometimes hundreds of meters in typical crystalline rocks and these should be at least 10m away from the canister hole. RM explained the respect distance in Swedish concept. SKB is concerned with potential reactivation rather than hydraulic properties, since these features could be reactivated and trigger the slip along the secondary fractures due to glaciation and deglaciation. According to SKB's preliminary study, single fractures with radii greater than 100m should be avoided from canister hole, because they could have an accumulated slip larger than the canister can withstand. Also, the respect distance should be the greater for larger features.

BF commented that we should be careful not to do too much modeling in the initial phase and we should set a proper goal at this stage such as a general understanding or a confirmation of the knowledge that we have. BF explained Nagra did not set up a near field model for low and intermediate level waste sites, although the data were available from an existing tunnel. BF pointed out that understanding processes is more important than fractures in sedimentary rock. AH agreed the danger of too much detailed modeling at the initial stage, but he also pointed out that the transport within fractures is necessary to run PA. MU commented that this will depend on whether we conduct PA and a possible way could be to make conservative assumption such as assuming infinite size and high transmissivity fracture. AH replied that POSIVA used this assumption and there was not enough retention for radionuclides and concluded not to allow these kinds of features, once or twice in a 200 meter section, to be near the deposition holes. MU commented that the crystalline rock in Japan could have high transmissivity features more frequently.

What levels of detail do you aim at for modeling (Conceptual, Numerical, PA) as the result of ISI?

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ABSTRACT

Numerical modeling conducted during the ISI phase should include modeling of both hydraulic and tracer tests conducted in boreholes. This type of modeling is specifically in support of site characterization activities and is not part of PA other than it may result in parameters that inform a PA model and definition of the conceptual models that underly the numerical PA models. In addressing the question of whether or not enough boreholes have been obtained to adequately characterize the site prior to construction of underground facilities, several types of analyses and modeling that begin to integrate site characterization and aspects of the PA process can be used. A relatively simple analysis is to quantify the data coverage through geostatistical analysis. Specifically, variogram analysis of the collected data (e.g., rock strength, fracture frequency, transmissivity, etc.) can be completed and then used to quantify the estimation, or kriging, variance at all locations across the site. Areas of high estimation variance are indicative of areas needing more site characterization. It may be possible to integrate both borehole and geophysical survey information into this type of estimation variance analysis.

Analyses beyond geostatistical approaches are necessary to explicitly incorporate any questions being asked of the data and to begin to incorporate elements of the PA. For example, knowing the spatial distribution of transmissivity only becomes an issue in the context of a groundwater flow model and any subsequent transport model. To focus the question of data sufficiency, numerical modeling using these data as input can be employed. This modeling does not need to use the full PA model for the site, but can use a sub-system model and proxy performance measures. Sensitivity analysis can be used to examine data sufficiency and locate additional boreholes. An example of this type of modeling is being used now to support long-term monitoring network design at the WIPP site.

MINUTE

Session lead by Anders Ström

Presented by Sean McKenna

SM argued that the goal of ISI is to demonstrate data sufficiency. He introduced his experience of long-term monitoring of the Culebra dolomite unit at WIPP. An area of 20km x 30km was studied by boreholes. He predicted the head and he was able to predict the head at the points up to 5km from the measured borehole based on estimation of variance. A goal was set to lower the estimation variance of head less than 25m² within WIPP site which is 6-6km square. An area was identified where more boreholes are required. This example can be used as an analogy to ISI. However, this study only addresses heads and not addresses PA. Therefore, he conducted stochastic inverse modeling of transmissivity field conditioned to both measured head and transmissivity. This transmissivity field model constitutes the subsystem model of PA. He considered the estimated head and transmissivity at each model cell to be stochastic input parameters to the transport model and studied the sensitivity using rank

correlation coefficient. Transmissivities varies over 5 orders of magnitude. 136 realizations were produced and particle tracking was conducted to derive mean travel time for each realization. Correlation between mean travel time and transmissivity and head was calculated at each point. Regions where travel time is highly sensitive to transmissivity and head were identified and locations for new boreholes were proposed.

Questions and answers

RM commented that the correlation length will be much shorter (less than 25m?) in granitic rock. SM replied that the variogram on head in granites will be smoother and does not vary as much over great distances as transmissivity or fracture frequency.

KK questioned treating heads as independent values, since it depends on boundary condition and the permeability distribution. SM agreed that results will only be valid for the assumed boundary conditions and conceptual model of permeability.

KK agreed to start modeling at the early stage, or even before the characterization. Also, KK commented that primary issues at this stage are the large scale issues such as the boundary condition, recharge rate etc. but also having detailed model, like fractured network modeling, from the beginning has the value of adding knowledge and iterating from the beginning stage. And at that stage, what you need is the boundary condition, recharge rate, all those rather large issues, but you do need modeling at the beginning. SM agreed and added that some sort of models can be used to help better define site characterization; what direction it needs to go.

TD questioned how this approach can be reframed if this approach is applied to the clay site where the retardation is taking place at very detailed scale. SM replied that his approach can be applied to any scale of heterogeneity. Think of an analytical or numerical model as a tool that can help develop our understanding.

KA questioned the definition of ISI and MU defined "ISI" in this workshop is investigation from the surface, such as surface geophysics and surface drilling, rather than actual sequence of site characterization, since some program already has URL at the beginning.

BF questioned filling a gap with additional boreholes if the Culebra dolomite is the host rock or below the host rock, since drilling additional boreholes could alter the rock properties.

HTa pointed out the necessity to consider other types of uncertainty including the uncertainty of variogram itself to judge data sufficiency. HTa also commented use of various different types of information, indirect, or some qualitative data from geochemistry.

TD pointed out the need to consider the difference between barrier part and conductor part. TD pointed out that the Culebra dolomite is a conductor part and not a barrier part. In an ideal sedimentary case, the host rock is rather homogeneous and highly continuous and can be characterized with high confidence by geophysical methods and one or two boreholes. This approach addresses the detailed scale model even at early stage in ISI, whereas in fractured rocks, the fractures are the conductors and much harder to detect. TD also pointed out as a potential issue at WIPP, the dissolution tongue which causes increase in transmissivity. This would be an unexpected event which could cause considerable uncertainty. SM replied that one criticism for the final calculations for WIPP was that there was not enough geology put into these transmissivity fields and he is now trying to put in the geologic conceptual model using

results of oil and gas drilling around WIPP.

MU questioned the role of the each scale of model. SM replied that he will explain the local scale around the repository in his following presentation and the role of the regional scale was very important to making the geochemical and hydrological interpretations consistent, since there was inconsistency between the geochemistry of the waters and the flow paths that were summarized at that time. TD introduced the scales in France; a regional scale incorporates the entire Paris basin, a sector scale which covers about a 20 to 30 km region and looks at roles of some faults, roles of potential closer boundaries, and the local scale which is the behavior of the host rock itself. The regional scale model uses boreholes from petroleum and the database. In the sector scale, ANDRA has an ongoing drilling program (that is just finishing up now) to better understand the encasing units and the boundary conditions. Concerning the host rock, ANDRA is starting another drilling program to look at the host rock properties. TD emphasized that “coherent” in French is an important concept which demonstrates the detailed scaled effect by showing its larger geologic manifestations through geochemistry, pore pressures, and everything else. Although the real containment in the host rock is controlled by angstrom pore sizes, hydrologic isolation is manifested in the regional scale model by the hydrochemistry and pore pressures, for example.

KM pointed out the performance measure should be carefully chosen depending on the safety allocation, such that Japan mainly allocated the safety on the engineered barrier and the groundwater flux can be more important in this case.

TD revisited the detailed scale modeling of crystalline rock issue. TD pointed out that we can get very detailed information such as conducting fracture spacings and frequencies from POSIVA logs, pump tests, advanced interpretation methods, and video borehole imaging. He also pointed out that spatial variability across the pluton can't be studied even at underground stage. RM introduced the SKB study on how much drilling and surface mapping would be necessary to adequately determine the true population of fractures. The result was that a very high accurate average behavior of DFN was obtained with fairly limited drilling and surface mapping efforts, when the Poissonian fracture distribution model was assumed for fracture system. These good results were due to excellent surface exposure of the granitic rock. TD pointed out the importance of non-stationarity. KK questioned the feasibility of detailed modeling based on a few boreholes, since the transmissivity of fractures vary over the magnitude of five orders and often fracture densities do not correlate with transmissivities. TD responded this will depend on the goal of ISI, such as whether one is aiming at ultimate numerical model of the site or one is trying to address an idea of block size. TD deems we can do the latter case, since we can understand the frequency of fractures exceeding a certain transmissivity value and we don't even need the flow model, if the boreholes are drilled in the right directions.

Uncertainties: which can be reduced, major breakthroughs, and how large at end of ISI?

UNCERTAINTIES

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ABSTRACT

The large uncertainties during ISI and ones that remain afterwards are those related to the critical issues and heterogeneities. Even if there is a significant focus on the critical issues during ISI the remaining uncertainties of importance tend to be on the same recurring issues. It may not be because of difficulty in studying these issues but because of their importance of those and that remaining uncertainties are still very significant. These uncertainties can be seen as almost inherent ones because the number of boreholes at any phase and the resolution and sensitivity of measurements is always limited.

Drilling more boreholes and performing more measurements reduces uncertainties significantly especially in the beginning of the ISI. The number of boreholes in the ISI phase could be typically four to ten with distances between them of 400 to 500 meters. Such widely spaced boreholes represent single, isolated samples of the heterogeneous rock (for all but the most significant regional discontinuities) and very few methods can characterize the volumes between the holes (seismic and large scale pumping tests, for example). When, however, the single borehole results can be coupled to other results, like surface based or airborne geophysical methods and geological surveys, an integrated picture starts to develop.

Typically new boreholes in ISI, but also in later phases, produce surprises, that is, not previously conceptualized or expected results. Then new targeted investigations are needed to resolve the problems, and an improved geologic conceptual model and bedrock structural model will be produced.

The geological conceptual model and the structural model with remaining uncertainties should be seen as evolving through all phases of site investigation, site selection, underground characterization, and repository construction. A strategy should be developed to meet potential adverse situations and conditions.

MINUTE

Session lead By Anders Ström

MU explained again the definition of ISI. ISI can be described as surface based investigations, such as surface mapping, surface geophysics, and limited number of deep boreholes (at most 3 to 10). AS confirmed that this definition is consistent with those of Scandinavia countries.

Presented by Aimo Hautojärvi

In crystalline rock, we have huge amount of heterogeneity due to fractures. Heterogeneity is not just hydraulic properties but also mechanical, geological, petrographical, mineralogical, thermal properties and so on. Let's consider the area of structures which bound the repository area, the surface area of the structure will be many km² assuming depth of 1km, whereas we

have only 10 penetrations with boreholes and the structure has heterogeneity. Thus our understanding is very limited. We need to understand this heterogeneity to predict discharge area, since the structure is channeled and discharge points are more localized rather than discharging all along the structure. Similarly, we need to understand meter or 10 m scale rock mechanical property to design the repository tunnel, rather than the core scale. This can be studied in underground and this is the remaining uncertainties.

Additional boreholes sometimes find more uncertainty and the uncertainty does not necessarily decrease as more boreholes being drilled. We need to have a good program to identify unanticipated uncertainty in early stage. The ISI stage does not need to understand everything if it is not fatal and the detailed fracture network should be studied in underground and during construction. Uncertainty can be reduced not just by increase in number of boreholes but by all the result from different discipline fit together and come to the integrated view. This integrated view is called the site description. The breakthroughs should be planned to be synchronized with program such as application.

Questions and answers

MU asked how to deal with more investigations if more boreholes may introduce more uncertainty and another problem. AH replied that we cannot get rid of uncertainties or surprises. In Finnish case, POSIVA encounters some features, which are not in their bedrock model, even after drilling 25 boreholes.

MU asked SKB whether they include small features in stochastic manner. RM replied SKB does not have any plan to conduct stochastic modeling including stochastic rock, since he thinks one will not be able to solve the shape problem.

AS introduced four examples of unanticipated events (expressed as surprises) experienced during site characterization at Forsmark. (1) They found a large outflow (1000 liter/min) at the depth of 100 or 150m along the percussion boreholes, (2) At the first 1000m long deep core hole close to the percussion hole, they found one of the least fractured rocks in Swedish program. (3) At the depth of 25m depth in the 3rd borehole, they found so called “porous granite” which could be a quite problem for constructability of repository. (4) In drill site #5, they found suspected/potential post-glacial movement.

RM pointed out that we should not only focus on boreholes nor geology, and that other disciplines like ecology is also important for PA and uncertainty from other components should be considered.

SS questioned about temporal uncertainty. AH replied that development of new fractures due to mechanical stress change during glacial cycles is possible, although no major change is expected, since the rocks have gone through many cycles. Also, repository construction could provide connections to fracture zones, all the boundary conditions such as hydrology are mostly time dependent. A large uncertainty is expected for melting of ice front, because of the possible large hydraulic gradient. Fracture fillings or minerals can change over the time and need to be studied.

Uncertainties : which can be reduced, major breakthroughs and how large at the end of ISI?

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ABSTRACT

There is often more than one conceptual breakthrough on a project. New data, new analyses, an outside perspective, and/or enough time to fully understand a new data set and its implications often precipitate conceptual model breakthroughs. An added issue with breakthroughs in conceptual models is that it does not occur overnight. It is usually caused by the slow accumulation of evidence that shifts the project away from the currently held conceptual model towards something new. Often this shift occurs in one area of the project prior to other areas. For example, data being collected by the site characterization portion of a project may cause a shift in the conceptual model describing a physical process, yet it may take a considerable amount of time for this shift in conceptual model to propagate through an organization and to finally be abstracted and captured correctly within PA models.

As an example of conceptual model breakthrough on the WIPP project in the U.S., the initial conceptual model of fluid flow within the host rock (salt) changed drastically from data obtained during the ISI to data obtained with higher resolution techniques from the underground facility. During the ISI, borehole and laboratory testing indicated that the permeability of the salt was 10^{-17} to 10^{-19} m², which was essentially the lower measurement limit of the testing techniques. Additionally, the conceptual model developed indicated that the brines in the salt only existed as isolated fluid inclusions rather than as a continuous phase along grain boundaries. This conceptual model indicated that rates of brine inflow due to construction and waste emplacement would be small and that in-situ permeabilities were large enough to dissipate any gas pressure resulting from degradation of emplaced wastes. As a result of these conclusions based on the conceptual model, further studies of gas generation and its effects on repository performance were terminated.

The conceptual model based on the ISI information changed drastically as the underground facilities were constructed. Excavations and boreholes in the salt host rock exhibited flowing brine weeps and underground based permeability testing resulted in a 10 order of magnitude range in permeability from 10^{-13} m² in halites and anhydrites in the disturbed rock zone (DRZ) to $< 10^{-23}$ m² for pure halites. The presence of flowing brine in the host rock led to new concerns on gas generation and its effects on repository performance and research in this area was renewed after a 10-year hiatus.

MINUTE

Session lead By Anders Ström

Presented by Sean McKenna

SM introduced the uncertainty at WIPP. SM explained that conceptual model breakthrough does not occur overnight but requires a slow accumulation of evidences. Often precipitated by new data, new analyses and outside perspectives. Also, time is required to fully understand the

current data. It often takes a long time for conceptual model changes to diffuse through an organization. As an evolution of the conceptual model, SM introduced the halite (the host rock) of WIPP. Up to 10 boreholes were drilled from the surface down to 600 meters deep and an original conceptual model was produced:

- Salt is “dry”; no interconnected porosity to conduct fluid flow,
- Brine only occurs in fluid-inclusions trapped within salt crystals
- Salt has homogeneous permeability

Interpreted permeability was 10^{-17} to 10^{-19} m² and was close to the detection limit of the surface based investigations. Later reexamination of these tests indicated none of these test provided data of sufficient quality. Conceptual model for the earliest PA assumed:

- No significant fluid flow in halite (Salado Formation),
- Salt has sufficient permeability to dissipate any waste-generated gas without significant pressure build up
- Gas generation studies within the WIPP program were terminated.

After constructing the underground facility, brine seepage was observed in new excavations. The quantity of brine was small, but indicated a continuous pore space in the host rock. More detailed permeability tests were run with new equipment. A single test sequence lasted almost 200 days. Heterogeneity in hydraulic conductivity was obtained such as pure halite has permeability of 10^{-23} to less than 10^{-24} m², impure halite 10^{-20} to 10^{-23} m², anhydrite interbeds 10^{-18} to 10^{-20} m², and fractured anhydrite interbeds were somewhat higher (10^{-14} to 10^{-17} m²). Thus approximately 10 orders of magnitude variation of permeability was recognized. A revised geologic conceptual model was produced, which includes thin layers of anhydrite interbeds of high permeability. The conceptual model was revised such that:

- Fluid flow to/from the waste storage room is strongly coupled with both gas generation processes/rates and with room creep closure,
- Important parameters for room-scale behavior include: interbed porosity and permeability, halite permeability, interbed threshold pressure, and disturbed rock zone properties,
- Permeability of salt is not high as was thought during ISI and gas pressure could build up. One concern is if pressure builds up higher than lithostatic pressure, fracturing of anhydrite interbeds could occur and permeability could increase,
- Even relatively small stratigraphic dip may have a significant impact on gas generation behavior,
- Gas generation became important again and the research program was resumed.

This is an example of how understanding during ISI changed with respect to how fluid moves from the host rock and this change in understanding greatly impacted the PA program in the WIPP project.

Questions and answers

BF commented that he can't understand why people came up with the totally homogeneous model, since fluid inclusions are well known, residual brine are well known, anhydrites are well known for salt deposits. BF also pointed out they should have drilled with air, and tested with gas if it is dry in order to keep a consistent concept. SM commented that this kind of analog study including later stage is important for planning ISI. BD commented we can avoid the pitfalls by having several alternative models.

TD pointed out that the diffusion model of the Culebra could be a nice example of an “event” as introduced by MU. SM explained that PA pointed out the importance of diffusion to meet the regulatory guideline at the very late stage in WIPP project and a series of tracer tests were conducted and demonstrated that diffusion was occurring and was an important process.

KM asked a question on the difference between geological conceptual model and PA conceptual model in WIPP. SM replied that there is a distinction between those two. The geological conceptual model is kind of a science piece of a project and understanding of the conceptual geologic model is outside of any direct regulations, but it is very important to demonstrate that the geologic conceptual model is well understood to be able to defend the PA and to make all information consistent.

Uncertainty in geological models with emphasis on geometry

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MINUTE

Session lead By Anders Ström

RM was inspired by discussion the day before and provided a complementary presentation on uncertainty in geological models to provoke discussions. RM began with statements (conclusions) as follows:

- Geometric uncertainties can be radically reduced with limited, targeted investigations. A problem is how much we can drill and still maintain the host rock performance.
- We have to accept some uncertainties because we can never address them completely or it is not worth for the effort. Examples are:
 - Large (single) fractures and very small fracture zones. We will never know their locations and we need to treat them stochastically.
 - Thickness of deformation zones, since we will never be able to have enough borehole intercepts to gain statistically valid thickness estimation,
 - Locations of deformation zones are uncertain until we intercept with tunnels,
 - Especially in granitoid rock, lithologic boundary in 3D. This is perhaps not important unless properties are different.
- Confidence and uncertainty are different. Uncertainty can be perfectly known. Increasing confidence is more important than decreasing uncertainty.

RM presented various examples of geometric uncertainties.

RM showed undulation of faults and pointed out that this provides uncertainty on the location of intercepts. However, conceptual understanding of faults on how they are generated and how they appear could enable us to estimate the probability of finding them. RM showed the variation in thickness of fracture. Thickness considerably varies in single feature. If one is trying to determine the feature thickness from borehole data such as fracture frequency, rock type and alteration, one will never get same thickness. One needs to rely on non-unique interpretation (expert judge) due to insufficient number of data to allow statistical analysis. RM showed an internal structure of fracture zone and pointed out that it comprises of many strands and causes uncertainty on number of the zones. RM explained the DFN uncertainty on fracture sizes. Fracture size data are generally available from outcrop and regional scale studies (from remote sensing and geophysics), and importantly there is an empty window for the intermediate scale, which is important for PA. Though power-law interpolation is pleasing, there is no reason not to use other distribution, e.g. lognormal, in the empty window because it has some advantages too. RM made a proposal to estimate large-scale uncertainty (large feature) on dip using the small scale uncertainty (local fracture) on dip using Fisher coefficient (κ). RM explained how to address uncertainty in local position using fractal/geostatistics with conditioning to observed points. Uncertainty can be expressed as “probability clouds” based on a large number of realizations.

RM stated summary as follows:

- All major deformation zones will be detected if steep,
- Major deformation zones with gentle dips can be detected with reflection seismic + drilling

up to 1000m deep,

- Highly probable that some minor deformation zones will be hidden in the modeled volume,
- Propose to deal with these uncertainties using DFN model.

RM commented on blocks and domains as follows:

- Defining block requires no special efforts, since block boundaries are already defined by the zones,

RM finally pointed out that subjectivity (expert judge) is important with reference to Äspö hydrostructure model. The geophysical measurement provided insignificant signature for the certain feature, but it turned out to be highly conductive. This could have been predicted by the long term tectonic perspective.

Question and answers

MU asked a reason why the vertical features can be detected, since it is generally difficult by the boreholes to detect the vertical features. RM replied that they have large percentage of outcrop such as 50-80% and it makes easy to find lineaments and they conduct a dense geophysics. RM explained that they rather over-interpret the lineaments.

MU asked a clarification of the terminology of “major deformation zones” and “regional fracture zones”. RM explained that the word, “deformation zone” is used to cover all different terminology on fracture, shear zones and sub-qualifiers are used to specify. Deformation zones are sub-divided into 4 classes, depending on the size ranging from regional scale down to the individual fracture. RM replied that “major” is equivalent to “regional”.

BF pointed out that if the site has sedimentary cover like in Northern Switzerland, it is not possible to detect steep features with geophysics and boreholes. RM agreed.

BD pointed out that characterizing fractures within the good rock (rock between the canisters and the nearest significant fracture zone) is more important for PA, rather than major structures which have little retention. RM agreed on importance.

SM asked the possibility to use geophysical data to better constrain the thickness of the zones for the stochastic simulation. RM replied that he uses stochastic simulation using geophysics to find the shape of deformation zone. Any information on thickness can be included and uncertainty can be dramatically reduced. If the features are horizontal or gently dipping, geophysics work very nicely and we will be able to understand shapes, extent and sometimes thickness, whereas these are difficult for the vertical features.

KA asked the relationship between geometry of deformation zone and hydrologic properties. RM replied what he presented is purely geometric, since one has to describe the object in 3-D space prior to assign its properties.

KK questioned the importance of geometry, since all fractures are not necessarily conductive and some fractures are sealed. RM replied that SKB considers two issues: 1) the long-term stability issue connected to future glaciations and 2) the constructability issue, since we do not wish to put canisters within deformation zones. We need to know 1) in order to calculate available volume for repository. KK asked the necessity of repository design during ISI. RM replied that we need to abandon the site (RM expressed as “showstopper”) if we don’t have sufficient space.

BD pointed out that faults are generally assumed to have sealing effect in oil industries and we

should keep this as an alternative to our conceptual model. RM replied we need to define geometry prior to assigning properties. TD pointed out that the context of total performance is extremely important, such as the more complete the EBS is, then the less exclusion distance we can assign.

MU introduced SKB's plan for defining timing (phase) of collecting parameters described in SKB TR-00-20. MU pointed out some parameters seem to be difficult to collect during ISI, such as:

- The location and density of local minor fracture zone (the length ranges from 10m to 1km)
- recharge/discharge areas (Hydrological parameters)

MU also pointed out some parameters can be obtained even during ISI such as:

- flow porosity, dispersivity if tracer experiments are conducted,
- Kd, diffusivity

MU asked participants to assess availability of the data during ISI and also to assess the uncertainty. AS pointed out that SKB is now planning to conduct the single well injection-withdrawal tracer test. RM commented that the density and the locations of the local minor fracture zone cannot be addressed during ISI.

MU compared the terminology of SKB and POSIVA on fracture/fracture zones of various scales and pointed out that SKB's terminology of the local minor fracture zone is somewhat too broad (the length ranges from 10m to 1km) and should be subdivided. RM replied that this boundary is being discussed in SKB. RM commented that fracture size distribution and fracture density can be determined but fracture location is difficult, and agreed that the table should be changed. AS pointed out that the table is updated in the new report, SKB TR-01-29 and MU announced that the table of TR-01-29 will be distributed.

**Modeling issues: Local scale model, calibration, boundary conditions, DFN,
Continuum**

**MODELLING ISSUES: SCALE (LOCAL/REPOSITORY/REGIONAL),
CALIBRATION/PREDICTION/VALIDATION, BOUNDARY CONDITIONS,
DISCRETE FEATURES?**

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ABSTRACT

Repository site assessment modelling can be considered in terms of three essential issues:

- a) VOLUME: Is there sufficient volume in the candidate site to locate the desired facility, considering exclusion zones related to significant geology structures?
- b) ADVECTION: What is the advective travel time distribution in the geosphere?
- c) DIFFUSION/SORPTION: How much radionuclide retention will occur in the geosphere for each of the radionuclides of concern?

As usual, the devil is in the details, and these simple questions can be answered at an infinite range of detail. At one extreme, modelling of hundreds of millions of fractures could be imagined, while at the other extreme, the entire answer is devolved to a simple pipe element. In the US radioactive waste projects, the bridge between these extremes is referred to as “abstraction”, which broadly refers to reducing processes to the simplest form which retains the most essential elements.

Scale Issues

- a) VOLUME: If there is not sufficient rock volume to place the repository, the rock mass will be rejected (or the criteria will be changed). Two scales must be understood to answer this question. First, what is the spatial pattern of the large-scale structures within which the repository must be laid out? Second, what is the rock mass which provides isolation from these zones? Both of these questions are 3D discrete feature issues, which can only be answered within a 3D discrete feature structural framework.
- b) ADVECTION: If the geosphere barrier is only considered in the region between the canister and the nearest major structural feature, then the scale of interest is well defined. Advection at the larger scale only becomes an issue if credit for transport processes and dilution at the site scale is to be considered.
- c) DIFFUSION/SORPTION: Diffusion and sorption are micro-scale processes, occurring with the interaction between solutes advecting through fractures and the immobile zones around/in these fractures. Scale issues arise in the characterisation of diffusion and sorptive processes at laboratory and experimental time and distance scales. How applicable are the derived properties at the scales of concern of repository safety?

Calibration/Prediction/Validation

- a) VOLUME: The prediction of the structures controlling repository layout and the geometry of the rock between the repository and the major structural zones from limited borehole and geophysical data is a major uncertainty. At the basic level, regional or generic information can provide “average” occurrence rates and properties for structures at kilometre, 100 meter and 10

meter scales. Geophysical information has increased in resolution and quality over the last 20 years, such that it is now possible to predict the geometry of structures at depth with some confidence. However, little effort has been put into quantifying the level of confidence, or the probability of undetected structures in the assumed repository block. Similarly, the volume of rock which provides isolation from the major structures is still not well understood. In particular, connectivity, compartmentalization, and the nature of transport pathways present significant uncertainties. Are models which neglect these phenomena while matching simple advective breakthrough curves “validated”?

b) **ADVECTION:** Advection is the most basic transport process, and in situ investigation would be expected to provide information to at least characterize advection. In general, models are first calibrated using simple experiments, and then are used to predict comparable experiments. If the prediction is successful, the model is considered “validated”. Can calibrated models be considered validated? Is it important to demonstrate predictive ability of advective transport models? How much confidence and realism is necessary?

c) **DIFFUSION/SORPTION:** The fundamental physics of diffusion is not really in question, and the range of material properties effecting diffusion is not very large. Sorption, on the other hand is an “equivalent” process used to describe complex chemical interactions. How useful is predictive modelling of diffusive processes? Can sorption models be considered “validated” when sorption itself is so much more complex than the models used? Are sorption and diffusion differentiating factors which even need to be considered in site selection? To what extent should initial site investigation and characterization be expected to address diffusion and sorption processes specific to the individual site?

Boundary Conditions

a) **VOLUME:** What boundary conditions are appropriate for evaluating the repository rock volume? The rock volume between the canisters and the nearest structure? Head? Flux? Current conditions? Worst case future conditions?

b) **ADVECTION:** Should advective boundary conditions be based on in situ measurements, symmetry “non-flow”, and topographic “constant” head? Are these concepts valid for repository suitability or safety? Are large scale flow models able to provide meaningful boundary conditions for the block scale analysis? What type of boundary condition is most appropriate at the block scale during initial site investigation? At the larger scale, what is the need for characterizing discharge and recharge zones, and quantifying dilution processes?

c) **DIFFUSION/SORPTION:** What geochemical boundary conditions should be assumed in evaluation of diffusion and sorption? How useful are in situ experiments at ambient thermal and geochemical (pH/Eh) conditions?

Discrete Fractures

a) **VOLUME:** Are there serious challenges to the concept that the occurrence and geometry of major structures controls the definition of repository siting volumes? Can the evaluation of geosphere retention at the block scale be reduced to the occurrence and properties of preferential pathways formed by fractures or fracture networks? If so, is EPM transport an important part of initial site investigation, or is the primary focus on geometry?

b) **ADVECTION:** Is it necessary to consider the distribution of advective velocities in a fracture plane? In a fracture network? At fracture intersections? Or, is a single “average” advection rate sufficient for site evaluation and safety assessment purposes

c) **DIFFUSION/SORPTION:** What geometries and immobile zone porosity properties and boundary conditions can be included in site assessment? Are there site specific immobile zone porosities, or are generic approaches with uncertainty more appropriate?

MINUTE

Session lead and Presented by Bill Dershowitz

BD addressed five modeling issues for ISI.

- a) Volume: Is there sufficient volume in the candidate site to locate the repository, considering exclusion zones related to significant geologic structures?
- b) Scale: What is the key modeling scale?
- c) Advection: What is the advective travel time distribution in the geosphere?
- d) Diffusion/Sorption: How much radionuclide retention will occur in the geosphere?
- e) Practical modeling considerations
 - Simulation of exploration activities using Bayesian updating uncertainty
 - Scale (Local/Repository/Regional)
 - Calibration/Prediction/Validation
 - Boundary conditions
 - Transport pathway approaches
 - Alternative modeling approaches

Concerning volume, BD pointed out that this is the first question needs to be answered, since the site could be rejected if there is not sufficient rock volume. BD also pointed out one needs to develop geologic conceptual model and hydraulic conceptual model with uncertainty during feasibility study and progressively reduce the uncertainties during each stage of investigation.

BD raised following scale issues:

- Are fracture zones part of the geosphere pathways, or a boundary condition?
- Compartmentalization is observed at many sites and possibly important. How is compartmentalization modeled?
- How well can the 50m scale geosphere be understood and modeled during ISI? BD considers that one could construct 50m scale model with uncertainty even before ISI using generic information. One can understand the reducing uncertainty using Bayesian updating approach.
- How can we extrapolate from ISI scales to pathway scales?
- What levels of uncertainty is acceptable at these scales and how do we quantify uncertainty?

BD raised following discussion topics on advection:

- Is flow model important for ISI? Is it sufficient to have boundary conditions or gradient?
- Does 50m scale advective transport model reduce uncertainty?
- Is flow and transport modeling necessary for confidence building?

BD raised following discussion topics on immobile zone:

- Do we model all possible immobile zone processes (diffusion into gouge/clay, altered zone) during ISI?
- How do we extrapolate in time and space from site characterization scale to PA scale?
- How do we quantify immobile zone uncertainty in ISI for modeling?
- Parameter uncertainty and process uncertainty. One needs to have alternative process models before ISI.
- How much model calibration and verification is required?

BD further presented Bayesian updating approach to judge how uncertainty could reduce by simulating exploration. Bayesian approach also allows to maximize the

cost/benefit by judging whether probability of “ success” increase sufficiently to justify expense.

BD presented issues on scales of concern as follows:

- Do you model site scale features to address exclusion zones or 50m scale model features or an integrated scale model in order to model entire the pathway from repository to the accessible environment?
- Boundary conditions to transfer between scales,
- Computational constraints and what should be ignored?

BD presented calibration and validation issues:

- When is “ good enough ” ?
- Can a calibrated model be validated?
- Should predictive modeling be carried out?
- What are appropriate criteria for calibration and validation? Can we say the model be validated if the calibrated value is at the extreme end of tested range?

BD presented boundary condition issues:

- The use of boundary conditions transferred between models at different scales can have a serious effect on model results. For example, a constant head boundary transferred from a regional model to a smaller model could over estimate the amount of water which can be delivered to the smaller model.
- One way to avoid this is to use integrated, multiscale models, in which the detailed model is nested within a simplified version of the larger scale model..

Question and answers

MS asked which geometric parameter uncertainty mostly affects the volume issue. BD replied that one can solve this issue by using the Bayesian approach. In this approach one will start evaluating all of the uncertainties at that time and also at the time of e.g., licensing. Then one should run modeling sensitivity studies to evaluate e.g., how much increase in number of additional boreholes will reduce uncertainty about the frequency of the fracture zones.

SM agreed the idea of using a Bayesian approach to site investigation, however he pointed out two aspects;

- 1) This approach could be subjective and the result could be biased if one claimed a large uncertainty at that time. The basic problem with the Bayesian approach is the difficulty in determining the appropriate prior uncertainty distribution.
- 2) As one conducts more characterization, one could encounter the information that drives the probability of success to zero.

TD added two aspects for the volume issue:

- 1) In sedimentary rocks, one has to consider diffusion and sorption as well as advection to discuss the volume issue and thickness of host rock,
- 2) Need for considering non-stationarity of fracture statistics.

BD commented that alternative conceptual models need to be considered and geological understanding as well as geophysical and hydraulic understanding could allow to obtain spatial trends and to understand different spatial domains.

MU asked when one should start uncertainty analysis, since there are too many assumptions that need to be made at an early stage and it will be difficult to judge the

relative importance. AH pointed out following aspects:

- There are limits where a site cannot be used as a repository site,
- AH ranks the volume issue as the highest one,
- At each stage, the general idea is to have the best understanding of the site, and admit that there are uncertainties in that, and then take further steps and go on with the program. Models are tools to develop our understanding, and to present our understanding. In different stages of the program, the weights between the different scales could be different. It could be possible that going from early stages to the final stages and underground stages of the site characterization, the importance changes somewhat from larger scale to smaller scales and more detailed modeling.
- Hydrochemistry cannot be addressed without description of the flow system at the site and there has to be this understanding, at some level at least, already at ISI stages.

MU agreed to have conceptual models at the beginning and asked what the best timing to start numerical modeling is.

AH replied that modeling with even zero data is useful, since it will provide an idea which orders of magnitudes we are interested in for certain parameters. AH stressed that any kind of modeling, numerical and analytical and kind of conceptual modeling is even so important to be carried out throughout the whole program after these feasibility studies to work out some issues and scope and really develop and target and focus our further characterization activities.

TD commented that the modeling should focus on addressing whether the site meets rejection criteria, such as sufficient volume question.

BD addressed the sorption and diffusion issue. BD pointed out that this issue is important if one is to have a safety case in the ISI stage, especially for argillaceous rock in which diffusion process is dominant. SM commented that within any program, there is a demand to sample and test the materials but this is a practical issue rather than modeling issue.

MU raised a question whether it is feasible to compare the model with actual discharge, at this stage. AH commented that discharge areas from the repository depend on the ratio of the overall gradient and small-scale variation in topography. In Finland, the long scale gradients are very low but local topography is somewhat high, and this creates very local flow regimes such that the transport length is often less than 1 km. BD commented that this issue is very important for safety case, even from the ISI and introduced that in the Yucca Mountain case, a geochemical model was used to evaluate discharge locations and back-calculate pathways from the repository. MU further asked whether there is field evidence to indicate the presence of a discharge area. AH commented that one possibility would be to measure the helium concentration which is produced by alpha decay of uranium in the bedrock. The production rate is constant and the helium concentration becomes higher as water goes deeper in bedrock and higher helium concentrations would indicate discharge points. KK commented that temperature distribution can be used as an indicator of discharge and recharge area.

What are the roles for conventional and safety assessment related modeling and how do these feedback with field activities?

WHAT ARE THE ROLES FOR CONVENTIONAL AND SAFETY ASSESSMENT RELATED MODELLING AND HOW DO THESE FEEDBACK WITH FIELD ACTIVITIES?

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ABSTRACT

SKB has started site investigations for a deep repository for spent nuclear fuel at two different sites in Sweden. The investigations should provide necessary information for a license application aimed at starting underground exploration. For this reason the site investigation data need to be interpreted and assessed into Site Descriptive Models, which in turn are used for exploring design options and for safety assessment studies. Site Descriptions are also needed for further planning of the site investigations.

Site investigations will proceed in stages, where the initial stage includes surface characterisation and drilling and exploration of a few deep boreholes at each site. A later complete stage includes drilling of about 10-20 deep boreholes per site. Site Descriptive Models are set up twice during each stage. The modelling work is performed in projects, one for each site. The Site Descriptive Model should be a multidisciplinary interpretation of geology, rock mechanics, hydrogeology, hydrogeochemistry, transport properties and ecosystems using site investigation data from deep bore holes and from the surface as input. The main components of modelling are:

- Identification of data
- Evaluation of primary data
- Three-dimensional modelling
- Overall confidence evaluation
- Documentation

The term interdisciplinary interpretation is used for the type of interpretation requiring interaction and consensus among the different disciplines. This is a major activity within site descriptive modelling. The different disciplines are to assess the suggested uncertainties and consider the feedback to the suggested geology, hydrogeology and hydrogeochemistry descriptions. In joint discussions overall confidence is assessed by:

- checking that all relevant data are used,
- checking that different kinds of uncertainty are addressed,
- checking if suggested alternatives make sense and if there is potential for additional

The confidence in the descriptive model is essentially a qualitative entity.

MINUTE

Session lead by Bill Dershowitz

Presented by Anders Ström

AS introduced the Swedish siting process. Feasibility studies were carried out at 8 municipalities and site investigation is being carried out at two municipalities at Östhammar and Oskarshamn. The siting decision will be made in 2008 to choose one site. Detailed

investigations will be carried out at 1 site. It is important to know about the siting process when talking about the uncertainty to be accepted.

Interaction among investigation, design and safety assessment is important, as well as coordination between two sites.

In the initial site investigations, a candidate area is given and the first step is to identify a site within the candidate area. After identifying a site, a few deep boreholes will be drilled as a compliment to the surface investigations. During the complete site investigation stage, a number of deep boreholes will be drilled and more surface investigations will be carried out.

Modeling has roles during feasibility studies (planning stage), during initial site investigations and toward the end of site characterization stage.

Planning stage

Three steps were taken in planning stage: 1) Parameter list (TR-00-20), 2) Updated parameter list (TR-01-29), 3) Site specific program (R-01-42, R-01-44, in Swedish). Safety assessment (SR97), Geoscientific and near-surface parameters (TR-98-02) and Requirements and criteria (TR-00-12) were fed into the program. The program addressed why and how we are going to do, but not necessarily how much. The requirements and criteria report presents a number of requirements on the rock and also, specific to Swedish repository system, such as rock composition and structure, groundwater composition, radionuclide transport, and construction and work environment. SKB clearly distinguishes between requirements and preferences. Requirements and preferences were produced through national dialogue and this provided good motives to SKB.

The latest PA, SR97 provides experience and a database and was used to explain all the requirements and preferences. Specific preferences are based on value ranges in recent safety assessment. A value out of range does not necessarily mean the site is bad, but means more it is more difficult and one has to do more analysis. Other uses will be to judge whether constructing repository is easy or not.

During site investigation

During site characterization, four modeling steps will be taken over 8 years. SKB is currently developing the first model version. Design people will make layout sketches based on this model and safety people will develop methodology and analyze specific functions in dialogue with design people. SKB will develop a much more mature model version called version 1.2 in the end of the initial site investigation stage. Based on the version 1.2 model, the design people will make a preliminary facility description and the safety people will conduct preliminary safety evaluation (not at all a comprehensive safety assessment). SKB will continue the investigation and produce a number of model versions. In the end of complete site investigation, SKB will produce the safety report.

SKB will have a formal review and feedback after the end of each of four steps. SKB will also have an international external review by the authorities/regulators in Sweden. There is also informal feedback built into the site organization, which is comprised of a site modeling group that includes the site investigators, and representatives from repository engineering and safety assessment groups.

The main product of modeling work during site characterization is called "site descriptive model." It is an integrated description of the site and its environments concerning the current

state of naturally ongoing processes. It comprises of 1) primary investigation data stored in database and GIS, 2) a site descriptive model developed with Rock Visualization System (CAD like system), and 3) a document providing a credible understanding of the site.

A site descriptive model is used for further planning of the site investigation such as providing recommendations to the investigation team, where to focus the next borehole investigation. Constructing a site descriptive model is a multi-disciplinary interpretation of the site. A representative of each of disciplines should work together all the time through the site characterization stage.

The site descriptive geological model version 1.2 should include:

- Description of the geological evolution
- A geometrical framework and geological parameter values describing the different domains:
 - Deformation zones
 - Rock domains
- Parameter description including spatial variability and uncertainty
- Alternative geometrical framework

AS introduced the regional scale geological model of Forsmark. Deformation zones are classified into high confidence zones, medium confidence, low to very low confidence to make alternative models. There are two ways to produce alternative models. One is alternative geometric frameworks and the other is alternative descriptions of properties within the same geometrical framework.

Toward the end of site characterization stage

AS introduced the roles of modeling at the preliminary safety evaluation. Objectives of the preliminary safety evaluation are:

- To determine, with limited efforts, whether the feasibility study's judgment of the suitability of the candidate area with respect to long-term safety holds up in the light of in-depth data,
- To provide feedback to continued site investigations and site specific repository design, and
- To identify site-specific scenarios and geoscientific issues for further analyses.

However, AS explained that these are quite limited effort at this stage of site characterization.

AS explained the table of analyses to be carried out in initial site investigation and complete site investigation. Analyses include thermal analyses, hydraulic analyses, mechanical analyses, chemical analyses, radionuclide transport analyses, and biosphere analyses. In the initial site investigation, a large portion of the analyses will not be carried out, but all analyses will be carried out in the complete characterization. For example, groundwater flow calculations (and salinity evolution) in superregional scale down to the local scale for historic conditions and present climate conditions are the task for SMG (site modeling group) and these will be addressed during initial site investigation, however those for future climate conditions will be conducted by SAG (safety assessment group) and addressed only during complete site investigation. At the end of the site investigation stage (late 2007), the safety assessment group will compile a comprehensive safety assessment called SR-SITE (Safety Report Site). SR-SITE will provide the basis for application to construct a deep repository at one of the investigated sites. SR-SITE will fully use the site data, will use the latest methodology and will include the latest R & D results.

Question and answers

BD asked the relationship between site modeling and PA modeling. AS replied that the site modeling will look at the present condition and the evolution. PA modeling will use the same set of models at the beginning, but can simplify the site modeling afterwards.

KM asked the role of the generic requirement and the specific requirement in case there exists different host rock. AS commented that the SKB's criteria are specific for Swedish crystalline rock and Swedish concept, and that these criteria should not be used for other context.

BD asked whether the judgment that the sites have sufficient volume to lay out repository can be established in the feasibility studies. AS replied that SKB judged that there is enough volume based on the feasibility studies, however AS pointed out that the volume issue is still a key question for the sites. BD further asked that a flow-chart going from site characterization to "can a repository be designed?" is missing. AS replied that the volume issue is one of the main targets when one makes these layout sketches and SKB will surely look into this issue. RM clarified that one of the main goals of the D-zero layout sketch is to see if they can squeeze in a repository, given the geometrical framework from the site model version 1.1 including the few parameters of relevance that can be extrapolated downwards, including their uncertainties. BD further asked how uncertainty will be treated in the volume issue such as a 70% chance that the site has enough volume. RM pointed out there exist two levels of uncertainty: 1) the first one is the exploitation ratio which means how many percentage of the blocks between the fracture zone is suitable for locating canister holes. This can be addressed by sensitivity analysis using stochastic fracture networks and calculate the probability of canister holes being intersected by fractures, and 2) the second is to determine whether there is enough rock block volumes within that framework. RM commented that the important uncertainties are i) suspected deformation zones (sub-planar geological structures) which are identified by various methods but their properties are not well understood. This is potentially important, since if suspected deformation zones are not real, this could significantly increase the available space for repository, and ii) to reduce the respect distance as much as possible, since this also provide an extra space for repository. To resolve i), SKB is currently developing a program to target the suspected deformation zones with percussion boreholes.

MU asked what kind of performance measures will be used for a site descriptive model during initial site investigation. AS replied that SKB is not using requirements or preferences as performance measures to provide feedback during site investigation, but the site descriptive model is used for understanding the site and to design further investigations. AS commented that Swedish regulators and international reviewers are interested in this aspect and ask SKB to specify the formal feedback and informal feedback built into the organization. SKB documents all the feedback such as a log file describing how the site modeling project provides feedbacks to the field activities.

MU asked how the uncertainty be treated. AS replied that SKB will discuss both what has been learned about the site for each discipline and also what uncertainty remains, and which version of the model to answer. AS explained that the uncertainty will be documented besides the site descriptive model in case the uncertainty is not addressed in the model.

MU asked how remaining uncertainty will be evaluated and how to provide feedback to the field investigation. RM commented that the reduction of uncertainty should be judged by the users (the design people or safety assessment people). AH commented one way to answer this question is to test ourselves through prediction and comparison with outcome and is important to conduct this kind of iteration throughout the whole program in all phases. MU pointed out

that constructing alternative models will be the good way to address remaining uncertainties. AS replied that SKB try to produce alternative models at each model version, however constructing alternative models will be rather limited in the first model version, since people need to spend more time to learn, new people start to involve and new projects need to start.

Accounting for the heterogeneity- needs in different disciplines (geology, hydrogeology, geophysics, geochemistry, rock mechanics) and reasonable expectations for accuracy, requirements at each scale, optimizing borehole strategies (objectives, location, etc)

**ACCOUNTING FOR HETEROGENEITY IN SITE DESCRIPTIVE
MODELLING-APPLICATION TO A GEOLOGICAL MODEL**

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ABSTRACT

Rock units can often be grouped together into *domains* with reference to a particular property. A geological *domain* in the bedrock can be composed of one or several rock units with similar characteristics with respect to a particular property. Two rocks, e.g. granite and gabbro, are considered as two separate domains with respect to physical properties, whereas two granitic rocks, e.g. granodiorite and tonalite, can be combined into a single domain, since their physical properties are similar. Units with similar hydraulic properties can be grouped into a hydraulic domain, irrespective of differences in other physical properties.

The concept of domains is primarily useful in the model building and is dependent on the aim of the modelling. The use of domains provide means to simplify a heterogeneous rock volume, at any given scale, into internally homogeneous volumes, with respect to a particular property or set of properties.

The use of domains is applicable to 1D (boreholes), 2D (geological maps) and 3D (geological models). Typically, domains are created in boreholes (single hole interpretation) and on maps independently to be combined and refined in 3-dimensionals geological models in a integrative and iterative modelling environment.

For geological single hole interpretation geophysical logs are not used in their primary form. Instead, transformed and interpreted versions are used, in which the results of several different logs are integrated. The methodology describing the processes of creating these logs is currently (October, 2003) being developed. *lithology logs* show the classification of rocks, based on the integrative interpretation of the natural gamma, gamma-gamma, and magnetic susceptibility logs. For this classification, determinations of the petrophysical characteristics of rocks are used, together with analysis of drill cuttings. *Fracture logs* show where, along the borehole, a number of geophysical logs have identified fractures or sections with fractured rock. The logs used are the caliper log, the sonic log and a number of different resistivity logs (SPR, normal resistivity, focussed resistivity, fluid resistivity).

MINUTE

Session led by Tom Doe

Presented by Raymond Munier

RM pointed out that this topic is very large and he will address only partially.

RM firstly introduced terms of “domains” and “units”. RM defined “units” as the smallest undividable volume or area in a model and depending upon its properties and intended use, and the qualifier such as lithological unit, hydraulic unit, structural unit, etc will be applied. RM also defined “domains” as a group of units which have similar particular properties. RM also

introduced anisotropy which means heterogeneity is different in different directions. SKB classifies rock volume into hydraulic conductor domains (HCD) which correspond to the fracture zone and hydraulic rock domains (HRD) which is the blocks between fracture zones, as well as a hydraulic soil domain (HSD) on top. RM showed examples of domains in various scales, starting from the whole Sweden, southern part of Sweden, the Forsmark site and outcrop scale. RM pointed out that heterogeneity appears to be scale independent and at least orientation of fracture sets appears to be similar on an outcrop scale and regional scale. RM explained the procedure of geological single-hole interpretation. FZI (Fracture Zone Index) which indicates potential deformation zone is semi-automatically calculated based on fracture and alteration data together with geophysics in a borehole. Then, the borehole is subdivided into domains. In order to produce a 3-D geological map of the site, SKB first take the geological map (2D) and create domains with simplification, but this simplification should be carried out under consideration the use of the end user. SKB merges 2D interpretation with single hole interpretation (1D) and produces 3D model.

RM pointed out the two issues:

- What is the critical size of “subobjects” (i.e. how small can a thing be and still neglect it and maintaining the performance or the properties of the model.)
- A risk for over-simplification.

RM discussed whether we have means of addressing this particular problem and how we can quantify it. RM showed an example of heterogeneity which is constituted of two properties A and B, and A and B equally occurs at 50% , but with different patterns (of wider alternation or narrower alternation). A pattern of very narrow alternation can be smeared out and regarded as homogeneous. The question is, how large, or how small can these be before one creates individual domains out of them. This must be steered by the end user.

Finally, RM introduced borehole program in Forsmark to account for heterogeneity. The zones are classified with uncertainty. The black solid lines indicate completely certain zones which are confirmed by tunnels or boreholes. The dotted lines indicate uncertain zones. In the Forsmark, three initial boreholes were drilled. Percussion boreholes were also drilled mainly for supplying water to the core boreholes. One core borehole is drilled entirely to deduce the decrease in anisotropy from outside into the lens of the shear pod. Other boreholes are planned to be drilled to see whether suspected zones (more or less linear patterns identified by an aero-magnetic map) exist. Plastic deformation is rather weak in the central part of the shear pod and it increases as closer to the boundaries, especially close to the major deformation zones. It appears that the folding of shear pod is scale invariant, since same folding pattern can be observed on outcrops. The question is how certain can we be of the shape of this thing at 500 m of depth.

Question and answers

MU asked whether domains will be defined for different disciplines such as hydraulic, hydro-chemical, mechanical properties or one common domains for all disciplines. RM replied that each discipline has its own domain.

MU asked whether there are criteria defining when a domain needs to be split. RM replied that when the properties within one domain differ substantially and it has substantial impact on any modeling that will be done within or including that domain. RM referred to the experience in Äspö. Although the pumping test and other tests indicate the existence of hydraulically conductive features, no geological feature was identified. In the later stage, it turned out to be that a very sparse swarm of thin, but very long fractures were the most hydraulically active

features. So, if this feature is known to exist, they should have created a domain to explain the hydraulic anomaly.

MU asked to which scale the domaining will be applied. RM responded that domaining can be applied to any scale. RM commented that domaining should not be done unless there is a purpose for the end users and sub-sequent modeling.

**BODA Claystone Formation (BCF) for HLW and Moragy Granite Formation (MGF)
for LILW Geological Disposals in Hungary**

MINUTE

Session lead by Tom Doe

Presented by Istvan Szucs

IS firstly introduced the current status of geological disposal program in Hungary. There are two main formations intended for site characterization. One is the Boda claystone formation for HLW disposal and the other is Moragy granite formation for low and intermediate level waste. In Hungary, there are four blocks of nuclear power plants. After the political changes in 1990, Russia restricted to receive back the high level waste in 1995, and Hungary had to start the geological disposal program. As a by-product of uranium mining, Hungary found a very good site. The Boda claystone formation is located to the west of the capital Pecs of Baranya County in southern Hungary. The yellow color shows the uranium mining area. In the last 50 years, more than 21,000 metric tons of uranium was mined. In order to mine this amount of uranium, more than 1000 km of boreholes were drilled and more than 1200km of tunnels were excavated. Therefore, the Boda claystone formation and the sandstone which contains uranium were very well characterized.

The ventilation shaft reaches the BODA claystone formation. The known area of the BODA clay formation is more than 100 square kilometer and the thickness reaches 800 meters. The depth of W-Mecsek URL is 1100m. Both the URL and uranium mining was terminated in 1999, due to the political changes and the uranium price change.

Hungary will start site selection process with the investigation from the surface in 2004 and select the site in Boda claystone formation within 3 years. Hungary selected the Moragy granite formation about 40 kilometers east of Pecs for low and intermediate level waste disposal based on screening process.

IS explained the seismic absorption tomography conducted using several boreholes in granite. The dynamic range of absorption tomography is between 2 and 200 (no dimension) and provides a very high resolution, whereas the dynamic range of conventional tomography is between 2000 and 6000 (no dimension).

The maximum distance between boreholes is 300m using an air gun as a source. If the distance is greater than 300m, blasting was used from outside. IS explained that he can correlate the tomography information with other parameters, such as the density of fractures, porosity, etc. by comparing with other measurements.

Question and answers

KK asked whether tomographic anomaly was correlated with hydrogeology. IS replied that it is possible to relate hydrology using tomography and core sampling. KK further asked whether IS found correlation. IS replied that some correlation was obtained, but the interpretation is not finalized yet.

CR asked whether IS calculated the shear modulus from intact rock. IS replied that it is calculated from the core sample.

BD asked the relationship between geophysical characterization and safety assessments for two

alternative sites. IS replied the work is in progress and they try to digitize different parameters. IS explained that understanding spatial frequency, dynamic ranges are important for digitizing parameters.

TD asked the spacing of boreholes for the tomography. IS replied that spacing of boreholes is usually 200m, the spacing of geophones is 3m inside borehole, the spacing of blasting is 10m and that the resolution of tomographic measurements is 5mx5m.

General discussion about Heterogeneity

MINUTE

Session lead by Tom Doe

KK asked whether the theme of this session is just heterogeneity or how much heterogeneity do we need to characterize during ISI. MU replied that the objective of this sub-session is to discuss the most important heterogeneity we have to characterize.

BF commented that a hydrologist will think hydrological heterogeneity plays major role because that is a pathway for radionuclides and a geologist might think geological heterogeneity is the most important, since the hydrology is influenced by the geology.

TD questioned whether there exists heterogeneity uncertainty or heterogeneity automatically means a large amount of uncertainty. RM responded that once heterogeneity is quantified, no uncertainty should be left. SM pointed out that if one knows the value at every point on the domain, then uncertainty has been reduced to zero, but typically we will never know that. So, we may be able to describe statistical parameters of heterogeneity, but that still leaves a large amount of uncertainty.

BD pointed out that the most important heterogeneity during ISI stage is geological structure, since this determines whether there is enough rock volume to layout the repository. If we know there is one structure every 500m on average, there is a lot of local heterogeneity within the average rate of structures. That really is the uncertainty that has to be reduced in order to determine whether we have enough volume to put down a repository.

MS pointed out that the heterogeneity is degree of spatial variation of the properties and features, and that the heterogeneity is very important if we can set a representative values for each domain, or if we should explicitly describe all complexity in the model. Heterogeneity is very important index to decide which model we should employ.

BD asked whether the best way to describe the heterogeneity within the domain is with a fractal concept of heterogeneity within the domain, a geostatistical concept, or a geological concept where there is some underlying reason. RM replied that fractal and geostatistics are basically same. RM explained that anisotropy is important at Forsmark and it helps to predict the heterogeneity in one direction with greater accuracy.

What are the critical measurements (e.g., large scale pumping tests, tracer tests)?

INITIAL SITE INVESTIGATIONS (ISI)

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ABSTRACT

In the context of the planning of an initial site investigation the following questions arise:

- What are the critical measurements (e.g. large scale pumping tests, tracer tests) ?
- How are data and conceptual models from other sites (including URL's) used ?
- Does information from generic sites reduce ISI characterisation needs (for retention parameters, for example) ?

The answer to this questions is that a correct answer cannot be given without knowing the boundary condition of the initial site investigation. It is therefore proposed to establish a stepwise approach for the initial site investigation.

Before doing so, it is necessary to clarify, as a first step, the needs of the end-users (e.g. in respect to safety issues, construction purposes or others). Based on this, the definition of the critical parameters the programme objectives and aims should be identified. An important general questions is for what is the ISI to be used (e.g. site comparison, site evaluation, real siting, political reasons, scientific study site or for a rock laboratory)?

Once this has been defined the following steps are recommended:

- Step1: Synthesis of preliminary site understanding; definition of an investigation and working programme; identification of possible uncertainties; setup of a QA/QC concept with well defined procedures.
- Step 2: Execution of the initial site investigation
- Step 3: Synthesis work of the initial site investigation
- Step 4: Refinement of a new scientific programme for further site investigation phases.

Various examples from Nagra's site investigation programmes in Switzerland, mainly from the high level waste programme (Opalinus Clay) were used to illustrate the presented approach.

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MINUTE

Session led by Tom Doe

Presented by Bernd Frieg

BF presented the Nagra's experience of initial site investigation. BF commented that there is no single critical measurement.

Step 0

BF introduced a step zero of ISI. BF presented the following points need to be considered to plan ISI:

- We need to understand the need of the end users at ISI stage, such as safety, construction purposes, or something else,
- Define the critical parameters for the ISI stage based on the aforementioned need, and
- We need to have a clear definition of the program objectives and the program aims. This requires understanding the bounding conditions such as dose limits and other regulations. In Switzerland, other regulations include the mining law and it is forbidden to build a repository where some kinds of ore deposits or natural deposits exist. Groundwater and environmental protection should be also issues.

Other general questions in step zero are what is an ISI for? Following examples are shown:

- Is it for site comparison? If this is the purpose, we have to conduct comparable amount of investigation at each site.
- Is ISI for site evaluation in general? If this is the case, an area will be selected for later detailed investigation,
- Is ISI for a given site?
- Is ISI for political reasons?
- Is ISI for rock laboratory site only?

BF added that "social-economic criteria can strongly effect every initial site investigation."

STEP 1

BF explained the Step 1 means to make a synthesis of the preliminary site understanding based on existing data. BF considers this would be easier in Europe, USA and in Japan, since a lot of information is available. After the synthesis, we need to develop a basic geo-scientific concept and need to come up with some predictions and assumptions, including basic data set, prior to investigation phase. BF stressed again to keep in mind "what is the aim of your investigation?"

BF presented options in sedimentary formations, Opalinus clay in Switzerland. Nagra produced a map where the Opalinus clay exists based on existing information. The map already includes some interpretation such as first priority area, reserve areas and the reserve option of the Lower Freshwater Molasse.

BF introduced the early concept of the Opalinus clay during Stage 1. At this stage, some aquifers above and below the Opalinus clay layer were known. However, concern at that time were whether some fractures go through the clay layer, whether some intermediate layers exist within clay layer, or whether there exist some minor aquifer. Therefore, advection, dispersion, sorption were assumed for intersecting fractures. Also, gas release and fracture formation due

to gas were concerned. Thus, we can draw investigation program already at this stage to address these issues.

BF explained hydrogeological mapping of 6600 meters of existing tunnels to check the inflows from the Opalinus clay. Result was that only minor in-flows with some damp patches on faults were seen and that no in-flow was observed under overburden of more than 200 meters. BF showed locations of existing boreholes. There are a lot of 3rd party boreholes, as well as NAGRA boreholes in Northern Switzerland. Nagra also compiled 2-D seismic data including 3rd party data.

The key questions from PA were:

- Does porewater in Opalinus clay form a mobile phase?
- What are the relevant hydrogeological scales and what are the relevant water conducting features?
- What are the governing equations of porewater flow in the site and which coupled processes may affect porewater flow? The coupled processes will not be taken into account in detail in the initial phase.
- The long-term evolution of hydraulic properties in the site?

BF presented how measurements should be selected according to assumptions on conceptual models. For the sedimentary rock, Opalinus clay, BF considers that fluid logging might not be relevant and normal integral transmissivity seems to be enough. If there exists a water conducting feature, hydraulic testing with small intervals seems to be appropriate. Fractured rock in which discrete features are localized can be characterized by fluid logging and packer tests, as well as the differential flow measurements. For up-scaling purposes, long-term packer tests and crosshole tests can be used. Transport properties can be conducted during ISI and not an issue. Nagra has once conducted a tracer dilution test in the Leuggern borehole at the depth of 1650m. However, tracer test is not carried out in sedimentary rock, since the host rock transmissivity is low and it takes long time.

BF explained an expected output as follows:

- Structure model:
 - Quantitative values of structure model
 - Information on WCF (water-conducting features) such as orientation, frequency, length, etc.
- Hydraulic model
 - Characterization of hydraulic properties of the different water-conducting classes,
 - Interval heterogeneity,
 - WCF transmissivities and average transmissivities,
 - Block scale effective K values,
- Advective transport properties based on tracer tests,
- Integration
 - Consistency checks with other dependencies based on independent evidence.

BF briefly introduced procedure to determine WCF transmissivities using packer test results and fluid logging results. The transmissivity value should be selected to define WCF.

BF continued explanation on Step 1.

- An investigation program should be defined according to the actual level of understanding,
- Working program should be developed based on preliminary concepts and models,
- Possible uncertainties in certain set-up and method should be identified,

- This will help us to consider how to reduce uncertainties in advance.
- QA and QC concepts with defined procedures can dramatically reduce uncertainties. BF pointed out that there is a risk to obtain meaningless number if they don't have QA/QC for hydraulic testing.

Investigation started with 2-D seismic and followed by 3-D seismic to reduce uncertainty on heterogeneity. The 3-D seismic surveys provide a resolution capable of detecting vertical displacements of less than 10m and are able to answer the question on fractures going through clay layer. The Neuhausen fault, the only feature, was identified. Except for this fault, the Opalinus clay is very homogeneous.

BF explained potential issues of hydrotesting and how Nagra resolved these issues. Issues were:

- osmotic flow
- swelling of clay minerals
- hydromechanical coupling (borehole closure, variable wellbore storage)
- temperature effects.

Nagra conducted design calculations taking into account of all these effects. A testing strategy was developed and was examined not showing different result from classical one. Also, in-situ testing was conducted in Mont Terri and laboratory testing using core was conducted. Analysis was conducted again and the working program was approved.

One of the outcomes of this was the establishment of special testing methodology after drilling with silicate mud. One needs to use silicate mud to drill through swelling clay to avoid swelling or borehole collapse. Potassium chloride solutions were skipped out because of the concern on potential chemical effects for water sample and core. Silicate mud has the disadvantage that if it doesn't pump around, it starts getting very sticky and clogs all possible features in the test interval. This was resolved by flushing with 70°-80°C heated NaOH solution for certain rather short time and then replace with synthetic porewater.

BF explained project management and quality control in Nagra. Project management and quality control in Nagra encompasses mobilization to have proper equipment, test designs, test performance, test analysis, and quality control. A very important component is test classification. Test classification will identify experimental error and skip the result with firm reason. Then interpretation will be conducted based on classification such as standard, or detailed, single phase or double phase. Separate documents will be produced by each packer interval and synthesis report will be produced in the end. BF recommend using this kind of approach, otherwise there are risks to run irrelevant test for the aims.

Step 2

BF explained the Step 2 (Execution of ISI). 3-D seismic was conducted and the borehole at Benken was drilled. Methods were implemented, results were obtained and analysis and interpretation was conducted. BF commented that the method, the results, the analysis, or the interpretation is less host rock dependent.

BF explained site investigation and geosynthesis.

The packer test data are transferred to the geosynthesis and combined with fluid logging data and long-term monitoring data. The data are reviewed in detail to check artifacts and two-phase flow properties. As part of the interpretation procedure, both the uncertainty range and borehole history is considered. Nagra normally conducts numerical simulation of the entire test sequence, forward calculations, inverse modeling using codes such as GTFM,

FLOWDIM, INTERPRET, MULTIFIT, KAPPA.

Step 3

The synthesis is a critical part and also the challenging part. Synthesis is implemented by comparing the independent parameters, such as hydrology and hydro-chemistry. One should also define the needs for further site investigation. This synthesis is host rock dependent. To conduct synthesis, one needs to really look into the data. Nagra conducted comparison of 3-D seismic with a walk-away VSP and these data nicely fit together. BF recommended using a walk-away VSP at Horonobe rather than normal VSP.

BF explained an issue on potential discharge area. There are two regional aquifers, the Malm aquifer above the Opalinus clay and the Muschelkalk aquifer below the clay. Isopotential lines for the Malm aquifer indicate discharge in the Rhine Valley. Additional boreholes need to be drilled to judge the flow direction. Faults and lineaments do not affect the isopotential lines. The flow direction within Muschelkalk aquifer is more uncertain.

BF explained how hydraulic data and hydrochemistry data were synthesized. Hydraulic conductivity in the Opalinus clay is very low. Water in the Opalinus clay was obtained by squeezing and leaching of drill core. The test results indicate very old water. When the transmissivity data are compared with H^2 , O^{18} , and ΔO^{18} profile, a nice fit was obtained by diffusion.

BF briefly mentioned the scales and hierarchy of structure elements in Opalinus clay. Heterogeneity can be seen in each scale down to micron scale.

BF finally commented that the study on coupled processes is needed for inter-disciplinary process understanding.

BF commented that Nagra is now in the last step of initial site investigation program, and is preparing to refine a new scientific program for the open questions or further investigations.

Question and answers

MS asked the range of transmissivity for Opalinus clay, and if there are any vertical fault with high transmissivity. BF replied that the range of hydraulic conductivity is 10^{-13} to 10^{-14} m/s and there is no high transmissivity feature. A main fracture zone can be seen in Mt. Terri, but the zone is sealed and can't see any difference from the wall rock.

How can the investigation methods be improved to reduce uncertainty? (Or are there novel methods to reduce uncertainty?)

USE OF NON-HYDROLOGIC DATA TO CONSTRAIN HYDROLOGIC MODELS

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ABSTRACT

Two examples are discussed, where non-hydrologic data are used to constrain a hydrologic model. In the first example, temperature data are used to discriminate models: Assigning lateral boundary conditions is a major point of uncertainty in model construction. We evaluate two models with opposing boundary conditions: mostly closed and mostly open boundaries. The two models show vastly different spatial distributions of groundwater flow, so we would like to find a means of choosing the more realistic model. Surface recharge is much larger for the closed model, but field recharge data are of too limited spatial extent to provide a definitive model constraint. Temperature profiles in 16 boreholes show consistent trends with conduction-dominated (linear) temperature profiles below depths of about 300 m. The open and closed models predict strongly different temperature versus depth profiles; with the closed model showing a strong convective signature produced by widespread surface recharge effects to the depth. The open model shows more linear temperature profiles, better agreeing with measurements from the field. Based on this data we can eliminate from consideration the closed model, at least in its present form in which surface recharge penetrates deep into the model. The second example involves the use of the surface tilt data to infer the fluid movement in underground. When fluid is produced from or injected into a reservoir, it causes volume changes in the reservoir, which in turn induce displacements on the ground surface. If a preferential flow path such as a fault zone exists in the reservoir (which is often the case in geothermal reservoirs) the flow will mostly occur along the fault. Observations of surface deformation can be used to estimate the distribution of the volume changes in the reservoir. For example, a vertical fault zone would produce a linear trough in the inverted image. The larger the volume change is at a particular location, the more fluid has likely moved in or out of the location. The distribution of volume change is tightly coupled with that of the reservoir flow properties: permeability and compressibility. Surface expression of such reservoir dynamics can be monitored by using high precision tiltmeters, GPS, laser level gages, and InSAR (Interferometric Synthetic Aperture Radar). Monitoring of the deformation at or near the surface costs very little when compared to drilling a large number of boreholes and instrumenting them with pressure sensors. This remote-sensing approach also provides an independent data of the reservoir dynamics that can be used to confirm/refute the reservoir model based on the borehole data alone.

MINUTE

Session lead by Tom Doe

Presented by Kenzi Karasaki

Before KK enters his topic, KK commented on the conceptual model breakthrough in Yucca Mountain. There have been five conceptual models over 20 years, and the current conceptual model is strikingly similar to the first conceptual model of 20 years ago.

KK introduced his topic is how to constrain hydrologic models using non-hydrological data. There is not enough data all the time. There is always uncertainty and the model is as good as the data. Therefore, we need help from non-hydrology data. KK introduced two examples. One is temperature data and the other is surface displacement due to fluid movement. These were studied in the MM project of the MIU program in JNC.

Temperature Data

Boundary conditions are one of the most important uncertainties. A no-flow boundary was assumed for ridges, the constant head boundary was assumed for the river. As to the lateral boundaries, two types of boundaries were modeled; one is a closed boundary (no-flow boundary) and the other is through-flow based on the large scale flow model. A recharge rate of 200 mm/year was indicated by a couple of measurements and this was considered to be too large. There are other uncertainties like fault properties and effective porosity.

Particle tracking was conducted and particle travel time was calculated as the performance measures. The closed model has longer path lengths and subsequently longer travel times by a factor of two. But there haven't been any other hydrologic data to indicate that one model is a better model than the other.

KK recognized that he needs to look at some temperature effects because the model boundary goes down to 3000 meters and the higher the temperature, the viscosity goes down meaning effective hydraulic conductivity goes up. If these are coupled, this could result in thermal convection or any other thermally induced effects.

KK showed the observed temperature profiles along the boreholes. DH-8 in the northern part of the modeled area showed a convex, facing upward temperature distribution, indicating a recharge zone.

KK conducted three cases to study; the first is coupled iso-thermal, the second is uncoupled, but considering the temperature rise will decrease the viscosity (which increases hydraulic conductivity) and the third is fully coupled thermal model. The result was that within the open model there was not much difference between iso-thermal and coupled cases. But between open model and closed model, average temperature of closed mode was 18°C, whereas that of coupled thermal in-flow model was 32°C. KK calculated the steady-state of the closed model and the reservoir cooled down too much because the recharge rate was too large for the closed model.

The temperature distribution for the open model matches better with the observed temperature distribution. This example illustrates how temperature data can be used to discriminate two different hydrologic models.

Surface Displacement

KK introduced surface deformation as another example of using non-hydrologic data. Surface deformation could take place when the fluid moves and volume changes underground. Surface displacement can be monitored by high precision tiltmeter, laser leveling, InSAR, GPS, or strain gauge.

KK applied to fluid injection conducted at the Okuaizu Nishiyama geothermal field in Fukushima prefecture in Japan. He used a tiltmeter with a precision of a few nano-radians. With the tiltmeter, we can obtain a trend in deformation in the x and y directions. 23 tiltmeters

were placed. The signal was that the geothermal power plant shut in geothermal steam and water for maintenance for about a month. Tiltmeter recorded change in trend right after shut-in started.

Very distinct signals of two humps were recorded at the same time in different directions along estimated fault zone. Volume change distribution was calculated by inverting the tilt distributions on the surface, assuming that volume change is due to the fluid movement.

KK explained the various methods to obtain displacement distribution data and the cost. Laser level measurements can provide less than millimeter accuracy, but it costs about \$100,000 for one shot at 50 locations. From InSAR (Interferometric Synthetic Aperture Radar) from airplane or satellite, one can combine ascending and descending path information and compile the interference ring.

KK also explained the tiltmeter application to the experimental fracture characterization site in Raymond, California. It is a granodiorite site and there is a loading or exfoliation fracture zone at depths of 30 meters and 60 meters. He packed off at 60 meters and did pumping and injection was conducted. Displacements were measured by tiltmeters during pumping. The pressures were measured in few boreholes. KK conducted inversion using 1) surface displacement and 2) surface displacement and pressure data for the volume change and permeability field. When he coupled the pressure, an assumption was made that the permeability was not a function of pressure, although the volume change in fracture zone took place. The volume change at about 30m depth was inverted, whereas the previous examples were at 1-2 km deep. Coupled inversion of the tilt and pressure data was used to reconstruct the permeability field.

KK mentioned that he could not use tracer tests to reduce uncertainty and he will not conduct tracer tests during ISI stage.

KK concluded that:

- Temperature data can be used to discriminate among different hypotheses on flow models,
- Surface displacement may be used to infer flow in a remote sensing manner.

Question and answers

SM asked whether the tiltmeter has enough depth resolution to understand the volume changes. KK replied that the tiltmeter data is the first derivative of displacement and don't have depth resolution and can have better control over depth if there is an actual displacement data.

TD asked if one needs to use unrealistic properties in model to fit the data when fluid moves very deep or very shallow. KK replied that a localized displacement will be observed if the volume change occurs very shallow and displacement in wider area will be observed if the volume change occurs at depth. KK added that if the fracture zone location is known, then fewer equations are required.

KA agreed the usage of the indirect data for flow model and asked the need for boundary conditions defined at the location where influence can be avoided and/or the need for considering hydrogeological knowledge such as the Tsukiyoshi fault in Tono forming no-flow boundary. KK replied that he used a larger model including ridgeline. The purpose of using temperature distribution was to discriminate two flow models, which assume different recharge/discharge. The closed model assumes 150mm/yr recharge whereas the recharge and

discharge rates in the open model were almost plus-minus zero. The conclusion was that a very small recharge into the deeper rock, and the most of the measured recharge is fed only into the shallower sedimentary rocks and running down the formation. KK also replied that the model is calibrated to the MIU-2 pressure data profile including high heads at the footwall of the Tsukiyoshi fault.

SM disagreed on not running tracer tests during ISI stage, since the tracer tests are invaluable for estimating the mass transport properties as well as the advective porosity. KK agreed that the tracer test will provide flow porosity and diffusivity, however he considers these will not be relevant for the Japanese siting criteria at this stage.

BD commented that generally hydrological models are pretty poorly constrained on hydrological data alone, and there is need for using complementary data to constrain the hydrological models. The complementary data include 3-D pressure field, which is the excellent method to understand compartmentalization and flow barriers, geochemical data, geophysical measurements such as 3-D seismics, AVAS, AVO, and geological data such as fracture data. KK disagreed on the usefulness of fracture data. BD commented two examples; one is the importance of fault internal structures to understand the granite hydrogeology, the other is correlation of fracture statistics spatial trend with the trend of permeability distribution. KK agreed the usefulness of fault internal structure.

How can investigation programs be designed to optimize uncertainty reduction?

DISCUSSION TOPIC: HOW CAN INVESTIGATION PROGRAMS BE DESIGNED TO OPTIMIZE UNCERTAINTY REDUCTION?

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ABSTRACT

A single answer to this question is impossible without reference to the requirements of the specific characterization program. Initial site characterization can vary greatly among programs depending on their regulatory requirements, program staging, and geologic medium, to name a few. For example, a program that is trying to rank several sites, without any requirement to site performance suitability, will have very different needs and uncertainties than a program that is trying to demonstrate that a site is suitable from a performance assessment perspective.

Uncertainty ultimately relates to the likelihood that a characterization program has reached a valid or invalid conclusion from the information. Although individual components – such as permeability, or fracture spacing, or identification of conductors – carry uncertainty, the ultimate uncertainty of importance lies with the decisions at the end of the process. If the goal is site ranking, one wants to be confident that the ranking is correct. If the question is site suitability, one needs to be confident that one has not accepted a site that actually bad, or rejected a site that is actually good.

This thinking leads to several principles for reducing uncertainty that may be applied regardless of program objectives. These are the following:

- 1. Clearly define program objectives.** Since the most important uncertainties are associated with program objectives, reducing uncertainty requires a very clear definition of those objectives. Unless program objectives are clearly defined, whether or not the characterization program is successful will be matter of chance. This means knowing what you are looking for and focussing uncertainty reduction on those issues.
- 2. Clearly define in advance the conceptual model to be tested.** Site characterization is a scientific program. It starts with hypotheses and the program should test those hypotheses. The uncertainties in the initial conceptual model should be defined, and the characterization activities should be clearly linked to resolving those uncertainties. Hypotheses might include ideas about fracture frequency or fault/conductor types, or the location and properties of a stratum.
- 3. Construct the characterization program using multiple lines of evidence for critical parameters and processes.** Depending on the program objectives, it may be impossible to define a process or parameter on the basis of one type of measurement. For example, the hydraulic conductivity measurements of a borehole do not provide a complete picture of the flow properties of the rock. Additional, complementary data should come from pressure interferences and geochemistry. For sedimentary beds, important constraints on hydraulic properties will come from anomalous pore pressures or chemistry. It is

important to recognize that one data type can have multiple interpretations, and independent lines of evidence are necessary to constrain data interpretations.

4. **Build in “reality checks”.** The incoming data should be regularly compared with the conceptual model for consistency. It is important to identify inconsistencies between the conceptual model and characterization results. Questionnaire 2 refers to the identification of the inconsistencies as “events”. Recognizing and resolving these events is critical to reducing uncertainty. The system should have simple numerical and analytical models to determine the implications of the incoming data. If the modeling or PA process is too long and complicated, an “event” may be recognized too late to do anything about it.
5. **Build in flexibility for program changes depending on outcomes.** Events need to be identified as soon as possible in a characterization program. The program needs to have some level of flexibility to allow for changes to respond to the conceptual model changes. These changes may involve location of holes, types of tests, or duration of tests. The flexibility needs to be built into the contracting and quality assurance systems. Without this flexibility, there is a danger that the data at the end of the characterization program will be inadequate to address the program objectives, thus leading to unacceptable uncertainties.

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Session lead and Presented by Tom Doe

TD firstly commented that he agrees points made by Anders Ström such as “clearly defining program goals and objectives” and “clearly define the conceptual models to be tested”. These are the way to reduce the uncertainty and to know what we are looking for, to know what we are going to test, and not to just have mass of data. TD also supported “Building in reality checks” and the idea of regularly gathering the entire team for the project from different disciplines to cross check to look at the data. TD supported “Build in flexibility for program changes”, so that we are not locked into a program when the data indicate the need for program change. TD also agreed with Kenzi Karasaki to construct a characterization program using multiple lines of evidences and stated that this is an extremely important tool for constraining models.

TD introduced TRUE Block Scale Project at the Äspö Hard Rock Laboratory in Sweden to address the characterization program using multiple lines of evidence. TD quoted Warren and Root (1963) which says “To develop a plausible reservoir model for an intermediate reservoir (this means fractured reservoir), it is essential that all the available measurements and observations be utilized, and the model must be consistent with the physical inferences obtained from actual reservoirs.” TD stated these words hold as true or more for what we are trying to do today.

TRUE Block Scale experiment studies the rock volume of about 200m by 200m. Seven characterization boreholes were drilled and the basics of the major conducting structures were understood by the end of three or four of these characterization boreholes. The last two boreholes were drilled to fill in a few minor zones and to confirm the conceptual model of the major conducting structures, as well as to conduct tracer tests.

The project used multiple lines of evidence. One of the best lines of evidence was pressure interference during drilling. Pressure responses were monitored at the packed-off sections when the new borehole is being drilled. Pressure responses occurred only at the specific monitoring sections when the new borehole intersects the certain features, which are connected to the specific monitoring sections. The connectivities of features at the scale of 30 to 40 m were mapped based on these pressure interferences.

Another useful measurement was the POSIVA flowmeter. The flowmeter has 10cm resolution, since the flowmeter is moved 10cm for every measurement.

A hydrostructure model of 200m block was constructed with high confidence and with quite high detail based on these measurements. A certain amount of compartmentalization was also identified. Major conducting features shows transmissivities of an order of $10^{-7} \text{ m}^2/\text{s}$. Background fractures are $10^{-9} \text{ m}^2/\text{s}$ or less, and the major bounding structures are $10^{-5} \text{ m}^2/\text{s}$. The POSIVA logs identified the detailed structures that were not observed connected between holes and these were treated as the stochastic background fractures.

TD explained how the water chemistry was used for integration. The structure 20 network, showed relatively saline waters, whereas the structure 10 and shallow features showed relatively fresh water. KA2511 which is located above 80 to 50 m above and across the main borehole array, is hydrologically not connected to any features in the block, except the deepest fracture zone and the shallowest fracture zone and it showed fresh water. Therefore, KA2511 is considered to be a separate compartment with different chemistry from structure 20 network.

TD explained the well test interpretation as the last example of integration of data. There are major advances in interpretation of well test data in the last 10 to 15 years. TD showed transmissivity-distance plot for TRUE Block Scale source zones. The plot was made by inversion and re-plotting of pressure derivative data. If the pressure derivative increases in time, it shows that the transmissivity is decreasing with distance, and if the pressure derivative tends to decrease with time, it shows that the transmissivity is increasing with distance. If several curves obtained from different borehole intersections look the same, it provides confidence that the different boreholes are sampling the same feature. A little variation at the beginning of the curve reflects the very local condition around the well, but they all then converge with time to a similar transmissivity value and then the transmissivity goes up at the end. If we know the diffusivity, the ratio of hydraulic conductivity to storage, which requires cross-hole testing, we can estimate distance. Uncertainty in distance is rather small, since diffusivity has generally much smaller range and the distance is based on the square root of diffusivity. The plot shows increases in transmissivity about 100 to 200 meters away and this will correspond to the major conducting structures, such as NE-2 and EW-3.

TD stated that the hydrologic characterization procedure for fractured rock can be summarized as a following work-flow:

- Flow log identifies conductors (or fluid logging for a quick look) instead of 1 or 30m interval packer test
- Image log and core define geologic properties of conductor
- Packer-piezometers are installed to isolate conductors
- Pressure monitoring during drilling
- Cross-hole hydraulic tests
- Tracer Dilution Tests
- Tracer Pretests

The POSIVA log gives much better resolution on the lower transmissivity structures that are important at the block scale.

TD introduced that a hypothesis being pursued in the continuation of the TRUE Block Scale project is if we can predict retention properties from the geology and mineralogy. If we can predict retention properties just by looking at core that would be a very nice thing.

TD presented an idea to drill paired holes during ISI stage. Using paired holes could resolve uncertainties as follows:

- 1) The first uncertainty is that the borehole penetrates the hydrologically dead part of the conductive fracture and may not capture all of the conductive features. Using paired boreholes could increase the chance to penetrate a conducting part of that feature. If there are the same flow log hits at the consistent places, we can be confident that these are the same conductors.
- 2) Another uncertainty resolved with paired holes is we can estimate distance in the well test analysis by being able to estimate diffusivity between the paired boreholes.
- 3) Another uncertainty about well test is the skin effects. If we have a second borehole nearby, we don't have skin effects.
- 4) Another uncertainty is transport properties and a second paired borehole would give an opportunity to run tracer tests and obtain either retention properties or simply flow porosity.
- 5) Finally uncertainty on connectivity will be understood by pumping one and monitoring the other. This could provide an estimate on fracture size which is one of the biggest problem for fractured rock, as well as compartmentalization and many other kinds of structural effects that we would not get from a single borehole alone.

TD concluded that we have made tremendous progress in fractured rock characterization in the last 25 years and we are in a position to use these tools very effectively for ISI.

Question and answers

BD pointed out that one can learn a lot more about rock mass by having a paired holes close to each other, but a lot less about the spatial heterogeneity across the site and there is a danger of a big volume of rock completely uncharacterized if there is significant variability across the site. TD agreed and pointed out that one could save the cost by drilling without coring.

AH disagreed on the paired hole idea, since one needs to drill several hundreds of meters just for access to the interested depth and it is better to go underground and do these studies there with ten or a couple of tens of meters holes. KK also disagreed since "no communication" between boreholes far apart is one information. TD replied that this issue will depend on the stationarity across the site. If the site is relatively stationary like Äspö, two boreholes apart will not add much information, whereas two boreholes close to each other could provide information on the connectivity and a lot of complimentary information. RM commented that having a pair hole will be feasible for SKB, since SKB plans to drill percussion holes besides deep cored hole. BD commented that multiple boreholes could provide a lot more information and questioned why not drill more percussion holes instead of expensive cored holes. TD commented that what he wanted to present was we already have tools to obtain block scale information even at ISI stage.

MU presented a block scale experiment conducted in granodiorite of the Kamaishi mine. By having rather dense borehole array (central boreholes were drilled 2m apart), compartments (zone A to F) were identified. MU thinks compartmentalization is potentially important for PA.

BF disagreed about the paired holes idea, since in northern Switzerland an initial basic concept for the crystalline rock (higher transmissivity zone only in upper part in crystalline and the low transmissivity for the lower part) changed after drilling at Leuggem where they hit high T

fracture zone at 1650m, at Siblingen where they encountered lots of high T (10^{-5} ~ 10^{-6}) fractures, and at Böttstein where they found only low T fractures. BF pointed out that there is a difference in outcrops/overburden such that the crystalline rock is covered with overburden in northern Switzerland, whereas crystalline rock is well exposed in Scandinavia. Nagra's site characterization concept is 1) conduct reflection seismic to locate major fracture zones, 2) drill boreholes in "star configuration", drill several boreholes from one place, incline the holes in the middle, 3) conduct seismic tomography between boreholes (penetration depth is 100-300m), and 4) propose a disposal area if the results are promising. TD commented that these could depend on how one sees the issues such that whether one targets intermediate fracture zones, or one target the host rock. Also this could depend on how many boreholes one plans to drill for bounding features and into host rock. BF commented that one can combine the purposes by having inclined boreholes and obtain information for both host rock and faults.

HTo stated that the pressure tomography is the one of the best technologies to identify the spatial distribution of properties during ISI stage and asked the feasibility. KK pointed out two issues for conducting pressure tomography during ISI stage; 1) the pressure signals can go any directions and the resolution might not be good, whereas the signals go straight in geophysical measurements. If the interpretation can be bound by fracture zone geometry, one can analyze, and 2) one may not see any interference, if borehole distance is kilometers. KK recommended conducting one or two good quality long term tests rather than doing many crosshole tests with mediocre or bad quality. KA commented that pressure tomography can be done, since RWMC, a Japanese organization, is doing a research for the crosshole electric geophysical survey with distance more than 500 meters and using several frequencies. They are combining the crosshole hydraulic test with geophysical measurement.

How are data and conceptual models from other sites (including URL's) used? Does information from generic sites reduce ISI characterization needs (for retention parameters for example)?

- Current status and survey technologies for siting projects in Switzerland –

CURRENT STATUS AND SURVEY TECHNOLOGIES FOR SITING PROJECTS IN SWITZERLAND

**A back analysis of Nagra's geosynthesis procedure
(HLW programme / Opalinus Clay)**

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ABSTRACT

Besides the assessment of highlights and challenges in the Opalinus Clay site investigations and synthesis programme the following statements made in the presentation:

- A systematic back analysis of the geosynthesis process can act as an optimisation tool for further siting strategy.
- Siting projects require tailor-made investigation programmes addressing the specific in-situ conditions, the host rock characteristics and the repository concepts.

The contributions of the different investigation methods of the Opalinus Clay programme in Switzerland (drilling, seismics, rock laboratory data and other studies) were presented. Generic programmes are obviously very limited to fulfill the needs of the end users in respect to siting, technical feasibility and safety demonstration.

Geosynthesis is the term given to a process where, starting from the field data and their interpretation, conceptual models and process models are developed. With integrated system models and consistency checks at least the geodata set can be verified and established.

Highlights and challenges of the Opalinus Clay programme were shown and the back-analysis of the data flow highlights both the priorities in the field programme and the synthesis of the geodata. The systematic back-analysis is based on the identification of key elements of the site investigations and the data analyses, as well as examination of the evolution in knowledge and understanding in the course of the siting process. The back-analysis can then also act as a valuable planning tool for future site investigation phases in respect to cost-benefit optimisation and prioritisation of overall project goals. A benefit for other siting programmes is the traceability of the synthesis procedure and the logical reasoning for in-depth site investigations.

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MINUTE

Session led by Tom Doe

Presented by Bernd Frieg

BF explained how various data sources contributed for each of three purposes, 1) siting demonstration, 2) demonstration of technical feasibility and 3) safety demonstration. Data sources are a) Benken borehole, b) seismic surveys in Weinland, c) Mt. Terri rock laboratory,

and d) other studies. For the purpose of 1) siting demonstration, mostly b) seismic survey is the most relevant and VSP at a) Benken borehole provided relationship with seismic survey. For the purpose of 2) demonstration of technical feasibility (that means stress field, rock mechanics, tunnel lining, long-term evolution), a) Benken borehole was the most relevant, c) Mt. Terri provided information, and d) other studies contributed to some extent. For the purpose of 3) safety demonstration as a barrier function, a) Benken borehole and c) Mt. Terri are the most relevant, and b) seismic survey and d) other studies contributed to some extent. Mont Terri rock laboratory plays important roles in the whole overall concepts, and also play a role in the future, if Nagra progress further on HLW.

BF explained the geosynthesis of Opalinus clay. Field data are Benken borehole, 3D seismic, Mont Terri rock laboratory and other sites, which include data from Site de l'Est, Toumemire, and regional studies. Firstly one will interpret field data such as geological, geo-mechanical, hydro-geological, and geo-chemical data. Then one should construct conceptual models and choose process models. The next step is to construct specific system models to study the undisturbed system, the disturbed system, and the long-term evolution, and to check consistency.

BF explained the Geodata set as an outcome of geosynthesis. The Geodata set includes all the models and the outputs to address all the issues relevant to the construction and operation report and performance assessment report.

BF explained the integrated system-models and consistency checks. Undisturbed system includes models of various scales and construction and operation. Construction and operation include the EDZ model which comprises of inner "damage" zone and outer "disturbed" zone. The model inputs are repository design, boundary conditions with in-situ stress measurements, petro-physical properties, geo-mechanical material laws, construction, and operation scenarios. Outputs are GeoDataSet (GDS), performance assessment, and design for construction.

BF explained a local hydrological model in undisturbed system. The model covers 10km x 10km area with 0.8km depth. The Benken site is located in the middle and the Neuhausen fault is included. The output is head distribution, hydraulic gradient, specific flux, and exfiltration pathways. The inputs include the host rock properties. Boundary conditions are provided from the regional hydrogeological model. Hydraulic properties are provided from packer test analyses.

Finally the long-term evolution will be evaluated.

BF explained conceptual models and process models. Many conceptual and process models are required to address structures and scales, deformation mechanics, and transport mechanisms. BF pointed out that the key part is not only to derive parameters out of investigations but also to understand the coupled processes. Different disciplines need to be integrated.

BF introduced further issues for siting and synthesis. BF listed the highlights and the challenges in field investigation that include packer testing and others. Very important thing in the highlights and the challenges in geosynthesis is the interdisciplinary communication.

Interdisciplinary communication should cover the three aspects such as 1) general understanding of host rock, 2) long-term evolution and 3) engineering feasibility and we have to understand a) scales and structure, b) transport behavior, and c) deformation behavior, as well as

coupling of these. Examples of coupling scales & structure with deformation behavior are porosity/compaction, diagenesis/geomechanical parameters, mineralogy/self-healing, and brittle structures/failure mechanisms.

BF explained confidence building by improving process understanding. The permeability – porosity relationship was cross-compared with results in the literature. Isotope profiles along the Benken borehole were compared with the diffusion model and groundwater flow model. Cross-comparison of gas threshold pressure, including Mt. Terri data, was also conducted.

Coupled processes on various scales were studied at Mont Terri, since these can't be studied at Benken borehole. These include gas test done between boreholes, cross-hole gas testing, and diffusion experiments.

BF explained the artifact analysis on packer testing. The key results from field campaign were K values in the order of 10^{-14} to 10^{-13} m/s, pore pressure was rather high in the beginning of recovery phase up to 3 MPa and poor match in the early time data. In the geosynthesis procedures, they tried to identify the key artifacts, and prove them, and revise parameter estimates. The conclusion was that the overpressures are still remaining and the concept to take overpressure into account is proved to be valid, and the K values were still in the same order of magnitude.

BF concluded that:

- Back-analysis of data flow highlights the priorities in the field as well as in the synthesis of geodata,
- Back-analysis is a valuable planning tool for future site investigation phases, cost benefit, optimization, prioritization of overall project goals,
- Back-analysis could also benefit for other siting programs because of its traceability,
 - Nagra has shown the traceability of the synthesis procedure and its logical reasoning for in-depth investigation.
- The key findings of Opalinus clay project is that confidence building by cross-comparison of results also with other results is an important point, and there is an enhanced demand for interdisciplinary work between site investigation, engineering, data interpretation, and also PA.

Question and answers

KK confirmed whether the 3MPa overpressure was known from beginning and then the artifact analysis was conducted or the result was reviewed afterwards. BF replied that there was a concept based on Wellenberg and underpressure was expected for the Benken borehole. A simple modeling exercise was conducted taking into account of topography and assuming more or less homogeneous properties. However, the result was that the pressure started subartesian, and then moved to artesian and it went down to 600m below ground level, and came back to 200m above ground level. KK asked the hypothesis on the genesis for those high pressures and under-pressures. BF replied that under-pressure in Wellenberg was due to rebound effect in tight rock after glacier. In Benken, it is due to compaction and it is still being compacted.

MU confirmed which information besides the site was transferred to EN2000. BF replied that a part of data including coupled process data such as gas test, diffusion test and EDZ properties. TD introduced the practice in France. ANDRA is heavily using information from the Mt. Terri

project, since Mt. Terri Opalinus clay is a similar Jurassic argillite from lower in the section and about 200 km southeast of Bure . AS commented that Äspö is extremely important, since Äspö is rehearsal for site investigation and an important database where site-specific information is not available.

KM asked how Nagra conducted the interdisciplinary communication to provide the goal for site investigation from safety assessment team. BF replied that the construction team, the performance assessment team and the geosynthesis team sit together and work strongly together the last 4 years. Each team consists of scientists from universities, contractors and others. Each team identifies the most important processes and transfer to the performance assessment team. BF pointed out that interdisciplinary communication is complicated if each team is sitting at different locations or different sites. Inside Nagra, Entsorgungsnachweis is given the highest priority and other efforts are removed from people.

Endpoint Session: What are the program goals of ISI? How does one decide the goals are met? How does one assure program goals are achievable?

WHEN IS THERE SUFFICIENT INFORMATION FROM THE SITE INVESTIGATION PHASE?

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ABSTRACT

SKB has started site investigations for a deep repository for spent nuclear fuel at two different sites in Sweden. The investigations should provide necessary information for a license application aimed at starting underground exploration. The geoscientific work is supposed to provide the broad knowledge base that is required to achieve the overall goals of the site investigation phase. The knowledge will be utilized to evaluate the suitability of investigated sites for the deep repository and must be comprehensive enough to:

- Show whether the selected site satisfies requirements on safety and technical aspects.
- Serve as a basis for adaptation of the deep repository to the characteristics of the site with an acceptable impact on society and the environment.
- Permit comparisons with other investigated sites.

Furthermore, the investigations are discontinued when the reliability of the site description has reached such a level that the body of data for safety assessment and design is sufficient, or until the body of data shows that the rock does not satisfy the requirements. These objectives are valid, but do not provide sufficient and concrete guidance. For this reason SKB has initiated a new project which should acquire concrete guidance on how to judge when the surface based Site Investigation Phase does not need to continue. The given project objectives are to:

- Develop the logical reasoning to be used for assessing sufficiency of the investigations.
- Identify different quantitative analyses to be used in support of an assessment whether sufficient investigations have been made.

Given the complexity of the task, it was found necessary to spend effort in more precisely define the problem to be analysed. Various system analyses tools including organised brainstorm and decision analysis have been used for this purpose.

MINUTE

Session lead by Hiroyuki Tosaka

Presented by Raymond Munier

RM expressed this is the one of the most tricky questions. In order to answer the question, “when do we have enough information?” RM introduced a graph, where the vertical axis is knowledge or lack of uncertainty and the horizontal axis is time or effort or money. Ideally, we define “sufficient” knowledge and we answer the question where we are. To achieve this, we have to define “What is sufficient?”, and we also have to find the means to “measure” if we

have actually reached that level.

RM explained a philosophical aspect. RM explained how knowledge would increase as time (investigation) proceeds such as 1) asymptotically increase with time, 2) increase with a steady pace, 3) jump after new batches, or 4) initially less and finally catch up. RM thinks a jump could occur between the version 1.1 and 1.2 and the difference between version 2.1 and 2.2 would not be significant.

RM explained a pragmatic aspect on knowledge. RM pointed out that we need to have a measure to judge whether the “obtained” knowledge at the deadline meets the “desired” knowledge.

RM quoted the site characterization objectives, “... site characterization should be discontinued when the reliability....reached such a level that the body of data for safety assessment and design is sufficient, or until the body of data shows that the rock does not satisfy the requirements”, and pointed out that this requirement is still loose and we need quantitative guidance.

RM pointed out that we need to clarify the clients (RM said “users” or “actors”.) RM explained the actors and the needs of each actor.

- Site modeling: needs to describe the uncertainties and confidence in that model,
- Engineering: needs to answer the question if it can be constructed with reasonable efforts,
- Safety assessment: needs to answer if the safety can be judged in the light of uncertainty and confidence in site description,
- SKB board: cost, time,
- International reviewers: Is there scientific basis for stated confidence?
- Authorities: Consultations, decisions, and
- General public: Is it safe?

RM pointed out that the last point is very tough, since we have to communicate our confidence in our work in such way that it is acceptable for the public.

RM explained the requirements (or show stopper) on the rock, as follows:

- The rock may not have any ore potential,
- We should not have any regional plastic zones within the repository unless the properties of the zone do not deviate from the rest of the rock,
- We must have room enough, both on a repository scale and on a canister scale, avoiding features that we do not want,
- The rock strength and the stresses must be such that we can actually build the repository,
- The groundwater at the repository level may not contain any dissolved oxygen, and
- The total salinity at the repository level must be less than 100 g/l.

RM explained the use of geoscientific suitability indicators and criteria at different stages by using an example of “no dissolved oxygen in groundwater at the repository level”. SKB is now at the site investigation stage and the site-specific information from the deep boreholes are sufficient to characterize the area. The geoscientific suitability indicators are the measure to make the judgment, and they are in this case Eh, Fe^{2+} and HS^- as indicators of the occurrence of dissolved oxygen. The criterion defines that at least one of the indicators, low Eh occurrence or occurrence of Fe^{2+} or occurrence of HS^- should be met, otherwise the site must be abandoned. He reminded that once we have written “Must be abandoned”, we cannot back away from that statement.

RM pointed out following critical issues which could relate to the investigation endpoint:

- Our ability to assess baseline conditions (such as seasonal or yearly variation) that are important to understand a certain process important for performance,
- Our ability to assess ore potential,
- Our ability to describe fracture statistics as well as individual fracture zones,
- Our ability to describe long term mechanical evolution (earthquakes etc.), and
- Our ability to describe the current distribution of the groundwater composition as well as its past and future evolution.

RM noted that a key issue is “Can an excessive amount of investigations impair the properties of a site?” Basically, this means “how much drilling is acceptable” and is called as a cheese topic (too many holes like Swiss cheese)

RM believes that we can accept an enormous amount of drilling as far as we do not intersect the repository level and yet we can significantly decrease many uncertainties on the geometry of the structures. RM pointed out two issues regarding panel layout. 1) The thickness of the fracture zone becomes critical, in case volume of the rock is limited. 2) The location of the fracture zone within the repository could significantly reduce the available rock volume. This problem becomes even more so intricate when there exist many zones intersecting at many angles, and if there exist the horizontal zones.

RM commented that SKB is targeting good rock with three cored boreholes during ISI, rather than the deformation zone. The aim with these cored boreholes is to find the showstoppers, like salinity, etc. The main reason for drilling cored hole is to study the rock mechanical properties at repository depth. An advantage of cored hole is to provide an opportunity to find surprises, such that the first borehole was very dry and very few fractures and they studied the rock properties of the core at the laboratory. Another surprise was the porous granite, and the question might not have been answered without core.

RM commented that SKB use cored drill holes only when it is essentially necessary to get sample of the rock at the specific position, otherwise SKB uses percussion holes because a percussion hole is not only less expensive but also much faster to drill.

Question and answers

YK asked whether we have to abandon the site if the rock doesn't satisfy the requirement. RM replied that there are showstoppers such as ore potential and we can't get rid of this with engineering or with more investigation, thereby we have to abandon the site. YK further questioned that scientists or engineer should provide some solutions to control the adverse conditions. RM replied that the issues other than showstopper can be compensated, but we can't compensate the showstoppers.

MS asked how many boreholes are needed to prove that there are no showstoppers. RM pointed out that there is also a limit for the number of boreholes. RM also commented that SKB is subcontracting a mineral exploration company to study how to address the potentiality of ore minerals.

Endpoint Session: What are the program goals of ISI? How does one decide the goals are met? How does one assure program goals are achievable?

**Discussion Topic 2: Endpoint -- What are the program goals of ISI? How does one decide the goals are met? How does one assure program goals are achievable?
Sedimentary Rock**

Thomas Doe

ANDRA

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ABSTRACT

The goals for initial site characterization of a sedimentary rock are relatively straightforward, and it is relatively simple to achieve them. The key things to show are:

1. **The host rock bed exists as expected.** The host rock has the expected stratigraphy, and it lies at the expected depth. This objective can be met by a combination of surface geophysics (especially seismic reflection) and drilling proceeded by good geologic literature work and field checking. Depending on the results of seismic investigations, there may be a need for checking structural features (faults) and their properties by direct drilling.
2. **The host rock has expected hydraulic, hydrochemical, and geomechanical properties.** This step can be met by borehole testing, sampling from cores, water sampling of encasing aquifers. Laboratory measurements of transport properties are important at this stage. A certain amount of longer term monitoring (1-2 years) is also helpful to identify very useful conditions like anomalous pore pressures.
3. **The hydrodynamics and boundary conditions are known to an adequate level of detail.** This step requires identification of possible water sources and discharge locations. Numerical modeling can help to guide how sensitive the characterization decision is to these considerations, and whether or not drilling and measurement is necessary, or approximations based on literature results are sufficient.
4. **Data are adequate to support application of success/failure/acceptance criteria.** A clear set of failure and acceptance criteria would be helpful for ISI. These can take various forms based on the program objectives. The criteria can be on individual parameters or on combinations of parameters that produce a desired performance. Either way, these criteria should be defined based on realistic scenarios in advance. The processes for judging these criteria should be specified as clearly as possible considering possible characterization scenarios. For example, these could include thickness and homogeneity of the bed (does it fall below expected range), presence of permeable fractures, etc.

MINUTE

Session lead by Hiroyuki Tosaka

Presented by Tom Doe

TD stated it is much simpler in sedimentary rocks to set goals of ISI and to decide if the goals can be met and achieved.

TD explained the major tools for sedimentary rocks. In sedimentary rock, the host beds are

usually extensively studied by groundwater studies and others, and large database including well logs, geological mapping and stratigraphy is available. A major difference from crystalline sites is that few very deep wells were drilled unless they are in mineral exploration zones. Another tremendous advantage is that experience and tools gained by the petroleum industry are available.

TD explained the goals for sedimentary rocks and these are a simpler problem. The goals are:

- To confirm the host rock bed exists as expected,
- To confirm the host rock has expected hydraulic, hydrochemical, and geomechanical properties,
- The hydrodynamics and boundary conditions are known to some level of detail, and
- Other criteria including being homogeneity, thickness, and relative absence of conducting features and other things that might be of interest.

TD explained the features which ANDRA and Nagra are focusing on:

- Diffusion-dominated flow system: The host rock in Bure is 130m thick clay layer, and distance to the biosphere is rather short, but it has low hydraulic conductivities such as 10^{-12} m/s and is a strong hydraulic barrier,
- Mineralogy is favorable to retention: clay has strong attraction for some nuclides,
- Geomechanics is favorable for stability: To have other minerals in the clay such as quartz, carbonate, other minerals provides stability.
- Properties favorable for fracture (EDZ) self-healing: This is a very growing area of research right now. Experiments at Mont Terri completed in the last year or two have shown that when water is present and the rock is subject to load, the permeabilities re-heal.

TD briefly explained the French program. In 1991, the radioactive waste act approved to find a laboratory site to start exploration. Between 1994 –1996, there was extensive 2-D surface seismic exploration at a sector scale, borehole drilling and testing. Based on these, a site was selected and 3-D seismic was conducted in that area and boreholes were drilled to monitor shaft construction. Shaft construction was initiated in 2000. In the Dossier Argile 2001, a sort of mid-term assessment was published. It included a performance assessment but it was intended to compile everything that was known up to that point and to identify the key issues. Underground testing will begin in 2004. In the meantime in 2003 and 2004, additional exploration holes will be drilled to investigate conditions near the shaft area and for boundary conditions. In 2005, the French parliament will receive a report from ANDRA that describes the status of radioactive waste disposal feasibility in argillite and in granite. And the parliament will also compare options for transmutation and surface storage. Thus, it is a major decision point for the French program.

TD briefly explained the geology of the Paris basin. The Callovo-Oxfordien clay in Jurassic was selected as a host bed. The key considerations made for choosing a site were to find a layer, at a particular depth, away from faults, and also of the appropriate thickness.

The Bure site was selected based on extensive seismic 2-D exploration of the area and three boreholes.

TD explained the stratigraphy of the Bure site. The host rock is the Callovo-Oxfordien (middle Jurassic) argillite, about 130 meters thick, and it is sandwiched between carbonate units of the Oxfordian and Dogger. The Opalinus clay is part of the Dogger sequence. The key criteria for locating this region was having the shale between 400 and 600 meters deep such that

it is deep enough to be away from the surface and yet shallow enough that it would not have problems with stability and closure. The other criterion was to be away from the faults. There is a small Tertiary graben and some faulting along the Marne river valley, as well as some more major crustal faults. The area immediately around the site is not structurally perturbed.

TD explained a hydraulic profile across the Callovo-Oxfordien shale unit. The pressures were measured with a number of Westbay installations in the carbonates and wireless transmission gauges in the argillite. The wireless transmission technology was adapted from the oil industry memory gauges by adding extended life batteries and improving the power management. Gauges have run as long as six years. The gauges are cemented in place and they transmit data through the rock. The signal is picked up at the surface. In Bure, the pressure measurements do not follow the theoretical line from conventional hydrodynamics. The argillite carries an excess hydraulic head that is about 30 meters above the overlying Oxfordian carbonates and 70 meters above the underlying Dogger carbonates. This overpressure can be explained by osmosis due to chemical potential gradients. The overlying Oxfordien aquifer is about 500 mg/liter total dissolved solid versus the underlying Dogger is about 4000 mg/liter. In the presence of a chemical gradient, the chemical gradient will cause in-flow into the shale that increases its pressure. Osmotic flow (chemical gradient driven in-flow) is balanced by an outflow that is driven by pressure diffusion. When this reaches steady state, this becomes a no-flow condition. TD also explained underpressures. This is observed in Wellenberg and clays in Canada. It comes from glacial unloading in impermeable rock. This indicates the rock is impermeable and the pressure lasted over 10,000 years. These phenomena are extremely important, since they reflect processes that act over large volumes of rock over time scales comparable to those required for geologic isolations of wastes.

Question and answers

HM asked who should decide the sufficiency of the ISI result. TD replied that managers and the budget people should decide. HM further asked how we can make a well-balanced decision including technical aspects. TD replied that we need to consider the risk to find out the evidence to conflict with the exclusion criteria and the uncertainty. AH commented that all actors should decide together, such that the safety authority should make their statement, the implementer should decide whether to spend more budgets, and the public should be directly or indirectly involved in the decision on whether the repository is acceptable.

KK questioned what the risk is in ISI. KK commented that it will be enough if one doesn't find the showstoppers.

BF commented that ISI is successful if predictions and assumptions made in advance are confirmed and the aims are reached. BF also pointed out that politics can stop the project, even if the project is technically successful.

TD agreed with AH on the importance of having the whole team to decide. TD commented that the project goal should be flexible and realistic that the site will meet the goal in a way of complementing the geosphere performance with the engineered barriers. BF agreed on setting the flexible goal, but pointed out that the goal should be so realistic that the site should survive the later performance assessment. BF commented that the rock salt will never clear the performance assessment, since there are risk that the whole salt layer could dissolve due to tectonics and faults.

Discussion on the table of SKB TR01-29

MINUTE

Session led by Masahiro Uchida

MU proposed to discuss the table of SKB's TR01-29, since availability of some data can be different in each country depending on, for example, the outcrop or sedimentary cover.

Geologic parameters

MU started discussion on geological parameters. MU pointed out that the detection limit for shear zone would depend on the outcrop/sedimentary cover, such that Japan has soil cover and Switzerland has thick sedimentary rock on top of crystalline rock.

AH commented that Finland has fewer outcrops than Sweden and has soil cover with average thickness of 2 to 3 m and this still makes it difficult to map fracture zones and minor fracture zones. Some part of the rock can be exposed by means of trenches, but trenches can not be left for long time and they have to be covered back. AH thinks that the large features of the bedrock structure like foldings and the correlation between geological history and features and hydraulic conductive fractures, for example will be difficult to study during ISI. AH commented that this would be very important to be understood and more work in the later phases of site characterization should be devoted to this matter.

TD commented that Tono or Mizunami is a good example of the crystalline rock covered with sedimentary overburden. TD also pointed out that the Japanese crystalline rocks have more weathered materials and are different from shield settings in Finland, Sweden and Canada.

MU agreed that the granite rock in Japan has a thick weathered layer up to 100m thick and this would make the characterization of minor fracture zones very difficult.

MS commented that the construction companies in Japan prepare an initial plan for a new tunnel based on lineament study. RM agreed on lineament as an important tool, however he reminded that lineament can only reflect the linear anomaly in the measured field and does not necessarily indicate deformation zone and it is crucial to confirm existence of structure. RM actually experienced that he got artifacts from clay layer cover at Forsmark. MU commented that all nuclear power plants have to evaluate the active faults in the vicinity of the plants by using lineaments and very often find other than deformation zones. TD stated that it is important for the Japanese program to establish the method to evaluate the probability of lineaments to be real geological structures.

MU commented that a 3D seismic survey is a good tool, although it is expensive. TD introduced the French case. ANDRA conducted 2D seismic prior to selecting the shaft location and conducted 3D seismic afterward, which can be regarded as being after the ISI stage. TD commented that 3D seismic should be conducted for a relatively small area and it is a matter of choice whether to characterize large region with less resolution or focus on a small region with higher resolution.

MU pointed out geometric parameters of local minor fracture zones will be difficult to detect if outcrop observations are not available. RM commented that the size distribution of the local minor fracture zone and large individual fractures are extremely hard to find, even when they are well exposed, since the outcrops are not usually large enough to observe the entire size of

the subject. SKB intends to treat the geometrical parameters of minor fracture zone and large fractures as statistical distributions and define their upper boundary as the lower truncation for the lineament map. RM suggested the Japanese program to extend statistical treatment of fractures to include larger features and analyze the consequence, rather than try to measure under poor outcrops. MU agreed and commented that his colleague has already conducted the sensitivity study.

MU asked the capability of 3D seismic to detect features in sedimentary rocks. TD replied that ANDRA uses 2D seismic to look for the largest discontinuities in the order of tens of meters of offset type features, whereas uses 3D seismic surveys over a few km around the lab site itself to find features with offsets on the order of few meters. Thus, the seismic survey is the primary tool to identify features and the secondary tool is the boreholes to confirm.

Hydrogeological parameters

MU pointed out statistical distributions of transmissivity (in the parameter group of stochastically modeled fractured zone, fractures plus rock mass) is not checked but this can be available by using POSIVA flow log. MS pointed out that fluid electric conductivity logging using a multi-rate pumping is also a powerful tool. TD stated that the fluid conductivity logging is a standard tool in ANDRA and that ANDRA is measuring the same hole with the POSIVA flow log. TD commented that the advantage of POSIVA flow log is having finer resolution than the fluid logging, since fluid conductivity log can't resolve discrete features when features occur relatively close together. The advantage of the fluid conductivity logging is not having its low-end transmissivity cut off. KK commented that the fluid conductivity logging is good for low inflow points unless there is high flow zone. TD questioned on the resolution of fluid conductivity log, since it is not clear how the head distribution and velocity distribution along the borehole are treated in interpretation.

MU changed the topic and asked about the techniques to identify recharge and discharge areas. AS answered that the recharge and discharge areas are identified based on topography during feasibility studies. Detailed new photographs and detailed topographical maps in a regional scale are made after entering the site investigation stage and hydraulic heads will be measured later in the stage. MU commented that in the country with flat topography, flow is governed by small-scale topography, but Japan is in more difficult situation, since Japan has high mountains and can have larger flow regions. AH provided a remark that recharge and discharge area in our discussion should distinguish surface water recharge/discharge area from the recharge/discharge area of the water which passed the repository. MU agreed and pointed out that Japan sometimes has confined aquifer and that the shallow flow system and the deeper flow system can be totally different. TD pointed out that this recharge/discharge area issue should be looked at from the whole hydro-dynamics of the flow system. TD also pointed out that the flow system in Japan can be quite complex such that a number of superposed flow systems with different depths and different recharges and discharge points are superposed. In such complex flow system, using hydraulic data alone can be very difficult to understand the flow system and one needs to use hydraulic surrogates such as hydrochemistry. KK commented that this recharge/discharge area issue is very important for ISI, since we can't significantly reduce uncertainties in later stage. TD commented that the surface drilling program can continue after ISI stage, for example, ANDRA is planning to drill additional boreholes to better understand boundary conditions.

KA asked the need for two-phase flow data (e.g. gas or methane data) in sedimentary rocks. AH

commented that 1) two-phase flow should be looked at if one wishes to better understand the water flow in soil cover, and 2) two-phase flow should be considered if the dissolved gases can be released due to depressurization.

BD pointed out that the tables are clearly designed for granite and there is a lot of other information necessary for argillaceous rocks, such as rheology, consolidation behavior, chemical degradation, interaction between pore fluids and matrix, multiphase behaviors, plastic behaviors, the confining layers, and overlying/underlying aquifers.

TD brought up the connectivity issue on stochastically modeled features. TD pointed out the discovery of dead end conducting fractures at Kamaishi. The connectivity issue is also related to the hydraulic compartment issue. BD added that the faults have internal structures and can behave as both conductors and also as flow barriers for flow across the fault. RM pointed out that we have lack of knowledge on the intermediate scale (50 to 250m) features, since this scale is too small for conventional geophysical method and too large to be mapped from outcrops. The uncertainty of the intermediate scale features should be analyzed. MU commented that flow barrier effect is potentially important, since it could divert the flow directly to the biosphere. RM commented that we need to be careful with available resources since it is not possible to study every deformation zone and channeling effect may need to be considered. BD responded that we only need a generic understanding and we will be able to include channeling, heterogeneity, internal structure and clay gouge, core for faults in a model. TD questioned if these parameters are critical for ISI decision. TD commented that the more important question need to answer is whether we have enough block size for repository.

KM commented that the recharge/discharge area issue is very important for NUMO, since the investigation area will be limited to the volunteer municipality (the average area is 10km²) and its vicinity.

TD commented that we can be confident with characterizing stochastic fractures by using POSIVA flow logging, borehole TV logging and the drill cores. We should also consider the methods to check, such as larger scale pumping tests on the intermediate scale features and detailed interpretation of well tests from this mid scale features to get connectivity data.

Compile goals, expected events, SI methods, level of details of GCM and PA, uncertainty, information to be used besides in-situ data, feedback.

MINUTE

Session led by Tom Doe

Laboratory contribution for reducing uncertainties (NETBLOCK experiment)

MU presented the NETBLOCK experiment. A granite rock block of 50cm edge dimension containing fracture intersection was used. Rubber gaskets with 5x5 windows for each panel are applied to all surfaces of the rock block. Constant pressures are applied for any combination of injection and withdrawal windows and the flow rates are measured. The transmissivities between the injection and withdrawal windows were calculated. The result showed that the combination of windows that include fracture intersections had the highest transmissivity. MU explained that these kinds of laboratory studies can be used to reduce the uncertainties.

Wrap up

MINUTE

Objectives/goals of ISI:

TD summarized his presentation and he pointed out that the major conclusion was that we have to consider site suitability criteria at all stages and that we should not proceed ISI unless we had some measure indicating the sites were suitable. How we measure the suitability of the site is a difficult issue and probably involves some kind of performance assessment.

What levels of detail do you aim at for modeling (conceptual, numerical, PA) as the result of ISI?

TD summarized that we need to address all scales in modeling.

SM commented that “Modeling of in situ tests” has the goal of reducing uncertainty and this requires answering whether we have enough data to reduce uncertainty. SM added the statement “Do you have the database to support the modeling that shows reduction of uncertainty?” TD commented that we need to add that we need to have clear set of techniques for reducing uncertainty?

AS commented that modeling should be performed all scales in ISI but limited in ambition. AS also commented that we should include an uncertainty description from the beginning.

Uncertainties -- which can be reduced, major breakthroughs, and how large at end of ISI?

TD introduced four bullets:

- Maintain alternative conceptual models for range of uncertainties
- Explicitly evaluate uncertainty before, during, and after ISI (through safety assessment?)
- Uncertainties due to boundary conditions must be addressed during ISI – recharge, discharge, hydrodynamics
- Reduce uncertainty using geochemistry

SM stressed the first bullet. If we develop and get stuck, it causes a lot of problems within the program. Therefore, it is extremely important to constantly consider and move forward alternative conceptual models.

AH commented that we should accept some uncertainties, since some uncertainties will remain and we can't do much about this. Also, some uncertainties will be quite large but still there is the possibility to make further steps and decisions on that. These uncertainties can be reduced in further stages of the program. TD agreed and pointed out that we need to prioritize the uncertainties to be reduced. TD commented that it will be difficult to describe the whole hydrodynamics with 3 or 4 boreholes, but we could reduce the uncertainty if we can get some geochemical samples showing residence time.

RM commented that it is quite easy to reduce geometric (fracture network) uncertainty since large outcrops will be available if we clean the outcrop and we can dig the sediment away if we don't have outcrop. This is a matter of cost and destroying the site and we have to balance the cost and outcome.

TD commented that we should add another bullet that simulated exploration in advance can help understand our uncertainties.

Modeling issues: local scale model, calibration, boundary conditions, DFN, Continuum

BD summarized the following bullets;

- Bayesian Approach to Successive Uncertainty reduction
- Boundary Condition Assumptions/Confirmation are very important
- Model prediction for confidence building
- Modeling of key hydrostructural features at all scales
- Use models to calculate probability of adequate rock volume
- Safety case modeling from feasibility study and ISI stages
- Study discharge area with helium and temperature
- Multiple lines of data to support modeling (geophysics, geochemistry)

RM stressed multiple lines of data and pointed out that integration between various working teams and various geoscientific disciplines is extremely important. The only means to achieve is to sit together. TD commented that the petroleum companies are also beginning to discover that geologist and reservoir engineers can work together and that improves the result.

MU commented we need to consider difference in surface and deeper hydraulics when we discuss recharge/discharge issue.

RM commented that the ecosystem description is an important part of PA and should not be forgotten. SR-97 clearly showed that the ecosystem is one of the most important parts and SKB is allocating large budget and effort to understand the present and future ecosystems.

What are roles for conventional modeling (e.g. groundwater transport) and PA and how do these feedbacks with field activities?

TD introduced the following bullets:

- 3D Hydrostructural Framework Modeling (SKB RVS)
- Ensure that all data are integrated to the modeling
- PA and Groundwater Transport both help integrate site understanding
- Multiple Modeling Iterations to Help Guide Site Investigation Decisions
- Models to Reflect Uncertainty

BD also summarized that this topic is “How do you ensure that the fieldwork collects the information you need for all the different kinds of modeling that you are doing and not just the mostly likely conceptual model but also the alternative conceptual models?”.

SM commented to add the phrase “sensitivity analysis”, since sensitivity analysis is a good feedback to site characterization. SM also commented that this does not need to be a full PA model and can be a sub-system model. TD commented that we will conduct PA before and after ISI and use sub-system model during ISI.

AS provided four statements:

- 1) Modeling has a role at all stages of site characterization, in feasibility study as well,

- 2) Site modeling performed in batches, in modeling versions, using investigation data packages can promote feedback in an ongoing site characterization,
- 3) In addition to formal feedback for modeling batches, informal feedback is also important. We should create an organization that promotes this kind of communication within site characterization. TD commented that this can be rephrased as “Management structures that promote frequent exchange of information.”
- 4) Safety assessment comes later, but still involves PA people and design people in the site modeling work.

RM commented that all users of the model must take part of the modeling work from beginning in order to see that they will eventually get what they hope to get and that they can steer the modeling so that it suits their need.

Accounting for heterogeneity – needs in different disciplines (geology, hydrogeology, geophysics, geochemistry, rock mechanics) and reasonable expectations for accuracy, requirements at each scale, optimizing borehole strategies (objectives, location etc.)

TD summarized as the following bullets;

- Key role of heterogeneity, non-stationarity, and multiple independent domains for site assessment and ISI strategy
- Optimize ISI to balance increased information from e.g., pairs of boreholes vs. spatial coverage
- Explicit ISI goals to evaluate heterogeneity

RM commented that the scale of the model will steer the degree of averaging within the domain.

What are the critical measurements? (e.g. large scale pumping tests, tracer tests)

TD introduced the following bullets:

- Multiple lines of evidence necessary (geophysics/geology/hydrology/etc)
- Design measurements to test hydrostructural conceptual model
- Understand advective and diffusive processes, requires diffusion and advection tests

TD commented that the critical measurement is the integration and not necessarily one particular test. TD also commented that measurements to obtain block dimension is critical during ISI and the POSIVA flow log is the best method. MU commented to include the fluid logging.

KK commented that the large scale (long term) pumping test is useful, during ISI, since this could allow us to average over large scale and other tests generally provide only local data.

SM stressed that we need in-situ tracer test to understand the advective and diffusive processes.

AH commented that rock properties and rock stresses, as well as thermal properties are critical to judge if the repository can be constructed.

RM commented that the show stoppers such as the free oxygen and salinity should be measured.

SM commented that a tracer test does not need to be limited to crystalline rock. TD agreed that the tracer tests in the encasing formations are quite important for WIPP and ANDRA.

KK commented that we can gain a lot of information by pressure monitoring during drilling of new holes. TD commented that head monitoring and pore pressure measurement are critical measurements. For sedimentary rocks, especially identification of anomalous pore pressures is extremely important and this is a critical measurement.

SM pointed out that a critical set of measurements during ISI is identifying the baseline conditions for everything, since some parameters will never be the same after excavating the shaft.

CR commented that measurement of in-situ rock stress condition is more critical than strength for long term stability of repository.

How can the investigation methods be improved to reduce uncertainty? (Or are there novel methods to reduce uncertainty.)

TD introduced a summary as follows:

- Use of temperature, geochemistry, deformation (tilt)
- Multiple lines of evidence
- Geological understanding
- New geophysical techniques (AVO, 3D Seismics, Electric Tomography)

RM commented that the multiple lines of evidences can be seen as an equivalent to multi disciplinary approach and it is critical for everything that we have covered on the entire workshop.

BD explained that AVO is a new seismic technique using different seismic attributes which are astonishingly good at resolving fracture intensity and fracture patterns down to tens or hundreds of meters scales. IS commented that AVO is a kind of processing method.

How can investigation programs be designed to optimize uncertainty reduction?

TD introduced following summary:

- Paired holes for connectivity and smaller scale hydraulic characterization – connectivity scale
- Transport aperture from tracer experiments?
- Flow wetted surface from sorbing tracers?

TD commented that we did not get a consensus on paired holes and corrected the phrase as “We have the techniques to do block scale characterization from the surface, if we wish to drill the holes and design them that way”.

AH opposed to use the flow wetted surface. AH stated that the flow rate is important and it is nonsense to conduct time consuming and complicated tracer test to obtain the flow wetted surface.

RM commented that it is important for program to be flexible to enables reflecting the results of

sub-modeling.

TD commented that we should consider the possibilities of using cross-hole technology (either hydraulic or geophysical), since this could add a lot more information.

KK commented that doing fewer but higher quality tests could reduce uncertainty better than a large number of lesser quality tests. TD proposed to conduct as much simulated exploration as we can so that we can better design the experiment, provide feedback to investigations and reflect the need from modeling. KK clarified that even after the careful design, the actual situation is the project is schedule driven and sometimes quality of the experiment is sacrificed and the uncertainty can't be reduced. TD summarized the discussion into 3 levels; 1) design a good test, 2) have flexibility during execution of experiment, and 3) have good feedback from users (modelers).

How are data and conceptual models from other sites (including URL's) used? Does information from generic sites reduce ISI characterization needs (for retention parameters for example)?

TD introduced a following summary:

- Generic data to support ISI design and initial assumptions of GCMs
- Provide hypotheses to test, and range of possible conditions
- URL as a testbed for ISI techniques and strategies

MU commented that the laboratory experiments like ENTRY could be used to reduce unanticipated uncertainties.

Endpoint: What are the program goals of ISI? How does one decide the goals are met? How does one assure program goals are achievable?

TD introduced a following summary:

- Goal is quantitative assessment of site suitability
- Increase confidence in site suitability – exclusion of exclusionary conditions
- Clearly define goals and test ISI programs against these goals
- Importance of QA/QC and tight management of ISI activities

No comments made for this topic.

Most important points from participants

TD asked each participant to present their selections of the most important points to see if the workshop could achieve a consensus on the major needs.

* Note: Statements are sometimes modified for clarity.

MU: Any kind of modeling can be useful to provide feedback from modeling to site investigation.

RM: Multiple lines of evidence.

KK: Multiple lines of evidence and the goal of ISI is to understand the system.
KA: Integration of communication.
MS: Exchange of information from international group, which has different environment.
Kim: Reduction of uncertainties is important, but also we have to accept some uncertainty.
SM: Any kind of modeling can be useful to provide feedback from modeling to site investigation “at all steps, or iteratively”
IS: Goal of ISI should be in a predefined framework.
HTo: Integrated understanding of the entire hydrological system including surface hydrology.
TO: Multiple lines of evidence
DL: Close data exchange/communication between experimentalist and modeler.
KH: PA people should be included in the ISI stage
KW: feedback from the PA and the integrated information
AH: Assessing the existence and suitability of rock volume
HM: Development of alternative models to achieve the feedback from model to ISI.
ST: To recognize the level of investigation method to underground and assessment of active fault in Japan.
HI: 1) Quantifying the uncertainty in the ISI is important from the viewpoint of pursuing the developing methodology for quantification. 2) Communication, especially with the regulatory body is important.
KS: 1) Integration and communication, and 2) the goal of ISI to understand the site itself.
YT: Communication with design and performance assessment people, especially concerning treatment of uncertainty.
???: This kind of workshop must improve public confidence and this kind of business.
???: Multiple line of evidence, because groundwater flow and underground event are themselves difficult to understand. So we have to compile or pile the data or the results to understand the underground events.
KM: Sensitivity analysis relevant for ISI is a good tool for stimulating the multidisciplinary communication and decision making.
SY: The goal of ISI is to understand the system and this will be done by multiple lines of evidence.

TD concluded the session and thanked everybody.

Closing Remarks

MU finally expressed many thanks to all of the participants. MU hopes this workshop will be fruitful to each country and contribute to each program.

Initial list of the workshop participants

AH: Aimo Hautjärvi	AS: Anders Ström	BD: Bill Dershowitz
BF: Bernd Frieg	CR: Chang-Ha Ryu	DL: Doo-Hyun Lim
HI: Hiroshi Igarashi	HM: Hitoshi Makino	HTa: Hiroyasu Takase
HTo: Hiroyuki Tosaka	IS: Istvan Szucs	MU: Masahiro Uchida
MS: Michito Shimo	KA: Kenichi Ando	KH: Koichiro Hatanaka
KK: Kenzi Karasaki	KM: Kaname Miyahara	KS: Kozo Sugihara
KW: Keiichiro Wakasugi	RM: Raymond Munier	SM: Sean McKena
SS: Shigeyuki Saito	ST: Seietsu Takeda	SY: Shin-ichi Yamazaki
TD: Tom Doe	TO: Toyokazu Ogawa	YK: Yongje Kim
YT: Yukio Tachi		

Conclusions from ENTRY2003 Workshop Session 2

Objectives/goals of ISI and desired output from ISI	<ul style="list-style-type: none"> ● Site suitability probability is the goal rather than ranking ● Objectives include understanding, reducing uncertainty, and ensuring that the site has a potential of success worthy of further investment
What level of details do you aim at for modeling (conceptual, numerical, PA) as the result of ISI?	<ul style="list-style-type: none"> ● All scales need to be addressed: Site, repository, local, block scale ● Clearly limited modeling scope ● Explicitly address uncertainty issues in modeling, including use of alternative models, sensitivity analysis ● Modeling of in situ tests ● Database to demonstrate uncertainty reduction ● Techniques for identifying key uncertainties and evaluating their reduction (e.g., sensitivity analysis, geostatistical methods, sub-system models)
Uncertainties -- which can be reduced, major breakthroughs, and how large at end of ISI?	<ul style="list-style-type: none"> ● Maintain alternative conceptual models for range of uncertainties ● Explicitly evaluate uncertainty before, during, and after ISI (through safety assessment ?) ● Uncertainties due to boundary conditions must be addressed during ISI – recharge, discharge, hydrodynamics ● Reduce uncertainty in geochemistry to better understand residence time, pathways ● Reduce uncertainty in geometric framework (balance between cost/boreholes and uncertainty) ● Accept uncertainties which will not be reduced in ISI, some will remain for further stages ● Wisdom to know the difference between key, immediate uncertainties and those which can be deferred

Modeling issues: local scale model, calibration, boundary conditions, DFN, Continuum	<ul style="list-style-type: none"> ● Multiple lines of data to support modeling (geophysics, geochemistry) ● Integration between technical teams, multidisciplinary modeling ● Bayesian Approach to Successive Uncertainty reduction (<i>Simulated exploration ?</i>) ● Boundary Condition Assumptions/Confirmation are very important ● Model prediction for confidence building ● Modeling of key hydrostructural features at all scales ● Use models to calculate probability of adequate rock volume ● Safety case modeling from feasibility study and ISI stages ● Study discharge area with helium and temperature ● Deep and surficial groundwater systems ● Ecosystem models including carbon circulation are necessary for safety and suitability analysis
What are roles for conventional modeling (e.g. groundwater transport) and PA and how do these feedback with field activities?	<ul style="list-style-type: none"> ● 3D Hydrostructural Framework Modeling (SKB RVS) ● Modeling role at all stages of site characterization ● Ensure that all data are integrated to the modeling ● PA and Groundwater Transport both help integrate site understanding (iterative, not continuously updated) ● Multiple Modeling Iterations to Help Guide Site Investigation Decisions ● Management to ensure informal feedback from modeling to investigation, and between modeling disciplines (including PA people, all other end users) ● Sensitivity analysis to support multiple conceptual models, driving data collection to discriminate between conceptual models ● Models to Reflect Uncertainty

Accounting for heterogeneity – needs in different disciplines (geology, hydrogeology, geophysics, geochemistry, rock mechanics) and reasonable expectations for accuracy, requirements at each scale, optimizing borehole strategies (objectives, location etc.)	<ul style="list-style-type: none"> ● Key role of heterogeneity, non-stationarity (spatial trends), and multiple independent domains for site assessment and ISI strategy ● Optimize ISI to balance increased information from e.g., pairs of boreholes vs spatial coverage ● Explicit ISI goals to evaluate heterogeneity ● Different model scales to address heterogeneity appropriate to each scale, upscaling between scales
What are the critical measurements? (e.g. large scale pumping tests, tracer tests)	<ul style="list-style-type: none"> ● Multiple lines of evidence necessary (geophysics/geology/hydrology/etc) ● Design measurements to test hydrostructural conceptual model ● Understand advective and diffusive processes, requires diffusion and advection tests (in situ tracer tests) ● Constructability tests (in situ rock stress, rock quality, strength, deformability, chemical stability...) ● Tests for exclusionary conditions (chemical, mechanical, spatial) ● Detailed flow logging to obtain repository volume assessment ● Geochemical sampling to support hydrodynamic model and test exclusionary conditions ● Seismic methods including tomography for hydrostructural framework, structure frequency, dynamic range ● Long term pumping tests (crystalline) ● Head monitoring during exploration activities (long term and systematic) ● Pore-pressure measurements, identification of anomalous pore pressures ● Baseline conditions critical
How can the investigation methods be improved to reduce uncertainty? (Or are there novel methods to reduce uncertainty.)	<ul style="list-style-type: none"> ● Use of temperature, geochemistry, deformation (tilt) ● Multiple lines of evidence ● Geological understanding ● New geophysical techniques (Advanced seismic processing methods, 3D Seismics, Electric Tomography,
How can investigation programs be designed to optimize uncertainty reduction?	<ul style="list-style-type: none"> ● New flow log technologies ● Cross-hole tests for connectivity and smaller scale hydraulic characterization – connectivity scale (block scale characterization from surface) ● Use of percussion holes to increase coverage ? ● Transport aperture from tracer experiments ? ● Parameterize transport processes from sorbing tracers (beta, FWS/q, advective distribution)? Multiple lines of evidence ● Design programs to support integration of sub-models ● Use analysis and modeling to support design of field activities ● Flexibility in field programs to meet changing or unexpected conditions ● Feedback between analysis/models and site activities

<p>How are data and conceptual models from other sites (including URL's) used? Does information from generic sites reduce ISI characterization needs (for retention parameters for example)</p>	<ul style="list-style-type: none"> ● Generic data to support ISI design and initial assumptions of GCMs ● Lab experiments such as ENTRY can reduce expected uncertainties ● International URLs ● Provide hypotheses to test, and range of possible conditions ● Test bed for ISI techniques and strategies
<p>Endpoint: What are the program goals of ISI? How does one decide the goals are met? How does one assure program goals are achievable?</p>	<ul style="list-style-type: none"> ● Goal is quantitative assessment of site suitability ● Increase confidence in site suitability – exclusion of exclusionary conditions ● Clearly define goals and test ISI programs against these goals ● Importance of QA/QC and tight management of ISI activities

Summary Bullet Points
Key Conclusions for ISI Sessions of ENTRY 2003
24 October, 2003

- Iterative Feedback from Modeling to ISI
- Multiple Lines of Evidence
- Goal of ISI is to understand the site
- Integration and Communication between disciplines (modelers, PA, experimentalist,)
- Exchange of Information between diverse international programs
- Reduction of Uncertainty, Acceptance of Residual Uncertainties
- Predefined Framework for ISI, incl QA/QC
- Understanding of total Hydrologic and Ecological System, esp Surface Data
- Characterize extent and suitability of rock volumes
- Assessment of Active Fault
- Methodologies for Quantifying Uncertainty
- Communication with Regulatory Bodies
- Improve Public Confidence
- Sensitivity Analyses to Support Decisionmaking and Uncertainty reduction
- **Thank You to Everyone for a Fruitful Workshop**

Notes: *1: "Event" means a jump in the evolution of the geosphere conceptual model(GCM) (Here, rather major increase in the level of understanding the site is intended, but minor increase can be included.)
*2:"Local Scale" refers to the scale where higher resolution model is applied, typically DFN model region between disposal tunnel and major water conducting features. This includes excavation damage zone.

Phases of investigation	Pre-Investigation phase (I)	Surface investigation and surface borehole phase (II)				Tunnel Excavation phase (III)	Underground testing phase (IV)
Dimensions of investigation A	Regional: 25km×35km (POSIVA, Olukiluoto) 15km×15km	“Initial Site Investigation” (II a)			“Detailed Site Investigation” (II b)		
		Regional:	Site scale, 1.2km×1.6km				
		25km×35km (POSIVA, Olukiluoto) 15km×15km (II a-1)	Surface Investigation (II a-2)	Few Boreholes Investigation c.a. less than 10 deep boreholes (II a-3)	Many Boreholes Investigation c.a. greater than 10 deep boreholes (II b)		
General goal, objectives and/or approach for each phase	(JPN) To select several preliminary investigation areas based on literature	(Japanese case) General goal -To select areas for detailed investigation based on initial stage site characterization at several areas.			(Japanese case) To conduct detailed site characterization to select the site for repository construction	(Japanese case) To conduct test in underground to prepare repository design and licensing by government	

	<p>survey avoiding disqualifying condition (active faults, volcano, high erosion rate etc.).</p> <p>B</p>					
	<p>(SKB) General siting studies for the entire country have been conducted as well as feasibility studies of a total of eight municipalities. The result was a number of siting alternatives. This was a solid base to proceed into the site investigation phase. At least two sites should be included in this next phase.</p> <p>(POSIVA) To select several sites based on literature survey to be classified into classes of suitability for further characterization (size, potential for suitable blocks, fracture density, topography, level of exposure).</p> <p>(ANDRA) To select an underground laboratory site that can also be used in the future as a repository is acceptable</p>	<p>(SKB) Initial investigation step will:</p> <ul style="list-style-type: none">– provide an initial basis for understanding (a number of key issues identified for each site)– preliminary evaluation of suitability at depth from limited number of boreholes <p>General objective:</p> <ul style="list-style-type: none">– Identify and select the site within a specified candidate area that is deemed to be most suitable for a deep repository and thereby also the part to which further investigations will be concentrated.– Determine, with limited efforts, whether the feasibility study's judgement of the suitability of the candidate area holds up in the light of in-depth data. <p>(Olkiluoto case + other sites) General goal</p> <ul style="list-style-type: none">-To select a few candidate sites based on initial stage site characterization at several sites. <p>Objectives ex.)</p> <ul style="list-style-type: none">-To collect data and understand each site to the extent of assessing constructability and safety-Key disciplines: geology and geophysics, hydrogeology, groundwater chemistry-Characterize lithology, structures, tectonics, various rock properties-Study hydraulic properties and groundwater flow regime, provide data for PA- Understand gw chemistry and its evolution, stability of chemical conditions at depth <p>(ANDRA) General goal</p> <ul style="list-style-type: none">-To select one candidate site based on regional screening-Provide data for Dossier 2001 and Dossier 2005 reports <p>Objectives: –Confirm host rock thickness and location</p> <ul style="list-style-type: none">- Locate possible faults or major fractures <p>(II a-B</p>		<p>(SKB) Overall goal is to obtain all permits needed to build the planned repository. A decision is needed before construction and detailed investigations (from tunnels) by municipality, government and environmental court. The “complete site investigation stage” is supposed:</p> <ul style="list-style-type: none">- To provide the broad knowledge base that is required to evaluate the suitability of the investigated sites for a deep repository.- The material must be comprehensive enough to:▪ Show whether the selected site satisfies fundamental safety requirements and whether civil engineering requirements are met.▪ Allow comparisons with other investigated sites. <p>Serve as a basis for adaptation of the deep repository facility to the properties and characteristics of the site with an acceptable impact on society and the environment.</p> <p>(ANDRA) - Establish properties of encasing units</p> <ul style="list-style-type: none">- Establish boundary conditions for regional flow- Establish groundwater chemistry of encasing units- Understand mechanical properties of host rock and rock stress at repository depth.	<p>(SKB) To be answered</p> <p>(III -B, IV-B)</p> <p>(ANDRA) Determine hydraulic properties of rock through monitoring activities in boreholes</p>	<p>(SKB) To be answered</p> <p>(ANDRA) Testing of properties and processes in host rock</p>
	(I-B)	<p>(DOE, YMP)</p> <ul style="list-style-type: none">•Surface geology•Mapping bedrock surfaces•Some boreholes to define Water Table	<p>(DOE, YMP)</p> <ul style="list-style-type: none">•More than 100 boreholes• ~10 deep boreholes• To define potentiometric surfaces, groundwater chemistry, fracture-fill chemistry, lithostratigraphy and matrix properties•To study shallow infiltration processes.)	<p>(DOE, YMP)</p> <ul style="list-style-type: none">• A series of shallow cored neutron boreholes to study infiltration processes.• Deep boreholes drilled for long term monitoring and geotechnical boreholes along surface projection of ESF prior to construction (ESF = Exploratory Studies Facility (URL))•Core analysis and borehole geophysics <p>(II b-B)</p>		<p>(DOE, YMP)</p> <ul style="list-style-type: none">•In situ stratigraphic locations•Sampling along ESF•Fracture mapping Detailed line surveys (DLS)•Local experiments

Event and investigation methods that caused the event	(Äspö/JNC)	i	ii iii iv v	vi	vii, viii	ix
		▽	▽ ▽ ▽ Evolution of investigation ▽ ▽			
Event ¹ in evolution of geosphere conceptual model (GCM), and the investigation that caused the event		i: <i>Estimated NE trending structure across Äspö from aeromagnetic, VLF and seismic refraction</i>	ii: Geologic survey : Estimated faults from fracture mapping iii: Geophysical survey : Estimated low resistivity zone from ground magnetic and electric mapping iv: The first drilling campaign: Divided Äspö island into three blocks; Äspö shear zone, northern block and southern block. v: Interference test during the first drilling campaign: Detected 4 conductors by interference tests at 2 boreholes	vi: Interference tests with all boreholes: Detected 10 conductors by 22 interference tests at 12 boreholes among 34 boreholes	vii: Understanding connectivity of structures and estimated undetected structures based on drawdowns during tunnel construction. Three types of responses (gradual, step, regional) to excavation which indicate pressure travel distance and/or diffusivities were observed. viii: Correction of flow porosities based on gw chemistry change during tunnel construction.	ix: Network and compartmentalization of conductors greater than 30m were identified with 6 of 200m long boreholes against 200m rock volume.(TRUE BS) A single fracture of 10-15m radius and its heterogeneity were understood with 5 boreholes.(TRUE-1)
	C (SKB) Good prospects of both satisfying the requirements on safety and engineering. Protection and being able to implement the deep repository project in practice. Based on surveys and desktop studies.	(SKB) i: Regional geological model only slightly changed from the regional model before start of site characterization – airborne geophysics, geological surface mapping.	(SKB) (Forsmark case) ii: Rock with unexpectedly low fracture frequency – core mapping iii: Porous granite is a potential problem – core mapping iv: Unexpectedly variable bedrock surface relief - drilling, ground geophysics, bedrock mapping v: Old water types near surface – surface water sampling	(SKB) Not applicable	(SKB) Not applicable	(SKB) Not applicable
	(POSIVA) Block concept of the bedrock structures in various scales (lineaments, target areas, blocks within block principle) I-C)	(POSIVA) i: Plastic deformation phases and lithological/ structural model from aeromagnetic (or Gefinex), VLF, horizontal seismic profiling (HSP) measurements and geological surveys	(POSIVA) Evolution of investigation (4 phases) ii: First phase Delimit rock blocks, locate surface expression of fracture zones by means of general survey (cf. IIa-1-C) and trench iii: Second phase Rock types, fracturing and fracture zones at depth by means of one deep (1000 m) borehole in anticipated most intact rock iv: Third phase Hydrogeological understanding by means of measurements in additional boreholes and at surface / shallow boreholes, data for individual fracture zones v: Fourth phase Understanding of ground water chemistry, stress state and improving hydrogeological picture by means of monitoring, sampling and long term pumping tests. Stress measurements were performed using the hydraulic fracturing method. (II a-2-C, II a-3-C)	(II b-C)		
	(ANDRA) Site selection based on criteria of depth, distance to faults, host rock thickness	(ANDRA) Event defined as the development of Dossier Argile 2001 Report Three holes drilled 1994-95 to confirm host rock depth and thickness Seismic studies to investigate faults over target area		(ANDRA) 2000 – drilling of pilot holes for two shafts 2003 – 7 FSP holes, 4 to Oxfordian 3 to Dogger, coring of host rock 2003-2004 – FRF holes to check faults and fractures, diffusion experiments	(ANDRA) 2000 – instrumentation of holes for monitoring shaft excavation effects (III-C)	(ANDRA) Start late2004

(IV-C)

Detailed description of investigation methods Investigation methods and amount at each event (with your assessment on the key methods marked with +(useful), ++(very useful), +++(extremely useful)) . If you think the investigation method is only useful for the specific condition, put notes for the method. If you are to adopt an improved method, please describe with blue letters.	<p>(Äspö/JNC) Satellite imagery, Air photo,</p>	<p>(Äspö/JNC) Airborne geophysics (magnetic, <i>EM, VLF, Radio metric</i>) <i>Ground geophysics (Gravity(1point/km²), Magnetic, VLF, Seismic refraction)</i> <i>Petrophysics (Density, Magnetic suscept., IP)</i> <i>Mapping of solid rock</i> <i>Fracture mapping study</i></p>	<p>(Äspö/JNC) <i>This example doesn't show the amount, pls provide the amount, too.)</i> ii: Geologic survey Outcrop study Trench iii: Geophysics : Electrical soundings Magnetic and radiometric profiles VLF and Wadi profiles Resistivity profiles Slingram and Magnetometer Seismic refraction Seismic reflection ○Drilling : <i>Describe the objectives of boreholes and describe how you decide the borehole locations taking into account of heterogeneity.</i> 14 deep boreholes (Core holes, drill length ca.500-1000m) 20 shallow boreholes (Percussion holes, drill length ca.100-200m) iv, v: The 1st drilling campaign:3 core holes(KAS02-04), 12 percussion holes(HAS01-12) 【the whole island】 Spinner log (++) Posiva flow log (+++) Interference tests (+++)</p>	<p>(Äspö/JNC) vi: The 2nd drilling campaign:4 core holes(KAS05-08), 5 percussion holes (HAS13-17) 【Southern part of Äspö island】 vi: The 3rd drilling campaign: 5 core holes (KAS09, 10, 11, 14, KBH02) 【Tunnel entrance moved to Simpervarp】 vi: Complementary survey: 2 core holes (KAS12,13), 3 percussion holes (HAS18,19,20) 【Structure study at southern Äspö island】 Spinner log (++) Posiva flow log (+++) Interference tests (+++)</p>		<p>(Äspö/JNC) ○ Drilling : • TRUE-1 • TRUE BS ○Logging • POSIVA flow log(+++) ○Dilution test ○Sorbing/Nonsorbing tracer experiment</p>
	<p>(SKB) Satellite imagery, Air photo, airborne geophysics, existing facilities, generic knowledge from previous site characterization</p>	<p>(SKB) SKB TR 01-29. An extensive and detailed site characterization programme has been constructed</p> <p>(II a-1-D)</p>	<p>(SKB) SKB TR 01-29 example: Bedrock and overburden mapping, ecosystems inventory Airborne geophysics and ground seismic Drill cores, borehole-TV Borehole testing: groundwater flow and chemistry, radar Airborne geophysics Geological mapping Seismics Drilling (percussion) Ecosystem documentation Cored drilling Borehole-TV Borehole geophysics Etc.</p>	<p>(SKB) In total 15 deep cored boreholes (700-1000 m): ▪ Base measurement programme in all ▪ Hydraulic tests 20 m sections in all ▪ 2 holes for complete chemical characterisation ▪ 4 holes for rock stress measurements ▪ 7 holes with hydraulic tests 5 m sections ▪ 4 holes with groundwater flow measurements ▪ 4 holes with interference testing ▪ a few single hole tracer tests About 30 percussion boreholes with base investigation programme.</p> <p>(II b-D)</p>	<p>(SKB) In planning (III-D)</p>	<p>(SKB) In planning (IV-D)</p>
	<p>(POSIVA) Satellite imagery +, Air photo ++, geological maps of Finland ++, existing survey results +++, combined with the Finnish map basis. Modern remote sensing methods with analysis and software (did not exist at that time).</p> <p>(I-D)</p>	<p>(POSIVA) Airborne geophysics (magnetic, VLF, EM, Radiometric Ground geophysics (Gravity(1point/km²), EM, VLF, Seismic refraction) Petrophysics (Density, Magnetic suscept., IP) Mapping of solid rock Fracture mapping study</p>	<p>(POSIVA) (Some very rough subjective estimates in personyears (py) are indicated) ii: First phase (30 py) Airborne and ground geophysics, geology, outcrop study, trench Electrical soundings, Magnetic and radiometric profiles, VLF and Wadi profiles, Resistivity profiles, Slingram and Magnetometer, Seismic refraction, Seismic reflection iii: Second phase (one borehole KR1 1000 m, 25 py) Rock types, fracturing and bedrock structures at intact rock Seismic tube wave, borehole radar, VSP, fluid resistivity and temperature, galvanic charged potential, borehole-TV iv, v: Third and fourth phase (KR2-KR6 2360 m, 40 py) Surface or near-surface hydrology and chemistry, seismic refraction survey, deep bedrock hydrology and chemistry, mineralogy, rock mechanical and thermal properties, VSP, Interference tests (+++), Posiva flow log (+++) (II a-2-D, (II a-3-D)</p>			

		(ANDRA) Literature Survey	(ANDRA) Seismic reflection (2D and 3D) to determine strata continuity and presence of faults with displacements greater then 5 m 2-D Seismic, several lines 15-20 km to identify stratigraphy and faults 3-D Seismic. detail over 2-km scale at lab site Standard Geophysical Logging Fluid conductivity logging Well testing for head and permeability (challenge of keeping holes open due to reactions of clay with water)			ANDRA) Fluid conductivity logging Groundwater sampling Tracer test on major productive zone in Oxfordian limestone Hydrofracturing stress measurements (concern about measurement quality of maximum horizontal stress in argillite host rock) Posiva flow logging (autumn 2003)	(ANDRA) EPG – embedded pressure gauges with wireless transmission Westbay piezometer systems	(ANDRA) Experiments in geomechanics, diffusion, permeability
GCM elements identified and characterized at the event <								

		(DOE, YMP, key elements) 1)Surface Infiltration rates and their distribution 2)Lateral flow in the unsaturated zone 3) Perched Water 4) Faults 5)Flux between fractures and matrix in unsaturated medium (I-E1)	(DOE, YMP) Scott et al. (1983) •identify problem •stratigraphy and structures •hydraulic processes •consequences of groundwater flow 1) 200 mm/yr. 3% enter as infiltration 2) lateral flow along interfaces (little vertical flow at repository level) 3) Potential perched water 4) Faults are open (II a-1-E1)		(DOE, YMP) Montazar and Wilson (1984) 1) 150 mm/yr 3% (0.5 – 4.5 mm/yr) 2) Lateral flow – diversion significant 3) Requires high matrix saturation before fracture conducts water - q _v ~0.5 mm/yr 4) Lateral Flow causes perched water that drain through faults to the saturated zone 5) Mainly matrix flow and little fracture flow in repository level and large lateral flow at the zone above. (II a-2-E1, II a-3-E1)	(DOE, YMP) Weeps Model (only fractures) No significant lateral diversion •Identified flow between matrix and fracture to be an important issue •Identify spatial distribution of Infiltration to be an issue. - need quantity estimate - topographic zones (II b-E1)		(DOE, YMP) Bomb pulse in ESF observed •Infiltration >1-2 mm/yr •Well-connected fractures •soil thickness <3m □Fast paths Fracture flow even when matrix is not saturated (non-equilibrium fracture flow) wetted fracture wells (1) Existence of high spatially & temporary variable Q: 5-10 mm/yr (2) little large-scale lateral diver above the repository level (5) Flow in fractures (non-equilibrium between fracture & matrix). Role of Fault in deep unsaturated zone not yet fully understood. (IV-E1)
	Local scale ^{*2} E2	(POSIVA) Not involved (I-E2)	(II a-1-E2)	(POSIVA) Detailed scale (intact block around deposition hole, 40 m) DFN model based on fracture mapping from outcrops, trenches and boreholes (II a-2-E2, II a-3-E2)		(Äspö/JNC) • Defined 10 geologic units and frequency of open fractures and average K was assigned for each unit (II b-E2)	(III-E2)	(Äspö/JNC) • Fracture networks of features greater than 30 m was identified. (IV-E2)
Uncertainty in GCM	Site scale			【Uncertainty reduced in event iv and useful method】		【Uncertainty reduced in event vi and useful method】	【Uncertainty reduced in event viii and useful method】	【Uncertainty reduced in event ix and useful method】
		(POSIVA) Nature of lineaments, structural properties of crushed zones, dip angles, depth and ending of structures.		(Äspö/JNC) • Locations and transmissivities of some major conductors [spinner log] (POSIVA) Positions and transmissivities of some fracture zones [double packer measurements, pumping tests, Posiva flow log] (ANDRA) -Stratigraphy of properties of host rock unit -Increase confidence in homogeneity of host rock unit -Evidence of hydraulic isolation from chemical contrast of encasing units and low permeability of well tests	(Äspö/JNC) 【Hydrogeology】 • Locations and transmissivities of other major conductors • Connectivity of major conductors (not all)[interference test]	(Äspö/JNC) • Location and transmissivities of additional conductors • Connectivity of major conductors • Fracture porosity of major conductors through modeling mixing ratio of gw chemistry.		
								【Uncertainty remaining at event iv】

F0	F1	(I-F1)	(II a-1-F1)	(Äspö/JNC) <ul style="list-style-type: none">• Locations and transmissivities of other major conductors• Connectivity of major conductors• Boundary conditions for flow and gw chemistry.	(Äspö/JNC) 【Conceptual model】 <ul style="list-style-type: none">• Connectivity of major conductors• Spatial extension of major conductors• Flow barrier effect of major conductors• 3D spatial distribution of gw chemistry 【Parameters】 <ul style="list-style-type: none">• Representative transmissivities of major conductors (Is model calibration against response during pumping test only way?)	(Äspö/JNC) <ul style="list-style-type: none">• Storativity of rock mass adjacent to major conductors to model mixing of gw chemistry based on flow model.• Groundwater chemistry data in average rock for modeling mixing ratio of gw chemistry.	(Äspö/JNC)
				(POSIVA) Locations and transmissivities of other major conductors (bounding features) Connectivity and extent of major conductors Boundary conditions for flow and gw chemistry, especially near-surface flow regime.			
				(ANDRA) <ul style="list-style-type: none">-Vertical fractures and faults in host rock (only vertical holes to this point)-In situ diffusion parameters in host rock-Detail characterization of encasing units over larger scale-Hydraulic head distributions over larger scale, discharge locations for encasing units-Investigations at this stage do not address the EDZ			
	Local scale			【Useful investigation to reduce uncertainty at this stage, Useful multiple lines of evidence】	【Useful investigation to reduce uncertainty at this stage】	【Useful investigation to reduce uncertainty at this stage】	【Useful investigation to reduce uncertainty at this stage】
				(Äspö and others/JNC) Ex.) -Pressure monitoring during drilling to understand connectivity. <ul style="list-style-type: none">-Rock strain measurement during pumping test to understand spatial distribution of flow path.- Mineral growth under different gw chemistry (such as calcite grows differently within fresh or saline water).	(II b-F1)	(III-F1)	(IV-F1)
				(POSIVA) More comprehensive hydrological and hydrochemical measurements and monitoring (small number of deep boreholes can be complemented with denser set of shallow boreholes, number of deep boreholes should be kept limited)			
				(ANDRA) Chemical and physical hydrologic data used to constrain transport velocities, use of isotopic data as natural analogs of long duration			
				-If you have ideas on novel/improved technique and/or use of multiple lines of evidence, please describe .(II a-2-F1, II a-3-F1)			
				【Uncertainty reduced in event iv and useful method】	【Uncertainty reduced in event vi and useful method】	【Uncertainty reduced in event viii and useful method】	【Uncertainty reduced in event ix and useful method】

	F2	(I-F2)	(II a-1-F2)	(Äspö and others/JNC) <ul style="list-style-type: none">• Fracture orientation• Fracture transmissivities [POSIVA flow log, fluid log]	(Äspö and others/JNC) <ul style="list-style-type: none">• Spatial variability of fracture orientation[BIPS log]• Spatial variability of fracture transmissivity [POSIVA flow log]		(Äspö and others/JNC) <ul style="list-style-type: none">• Fracture networks of features greater than 30 m was identified. with 6 of 200m long boreholes against 200m rock volume.(TRUE BS)• Heterogeneity of a single fracture of 10-15m radius was partly understood with 5 boreholes.(TRUE-1)
				【Uncertainty remaining at event iv】	【Uncertainty remaining at event vi】	【Uncertainty remaining at event viii】	【Uncertainty remaining at event ix】
				(Äspö and others/JNC) 【Conceptual model】 <ul style="list-style-type: none">• Fracture size• Spatial distribution of conductive fractures• Connectivity of conductive fractures• Compartmentalization• Channeling• Fracture intersection• Spatial variability of aforementioned parameter• 3D distribution of gw chemistry• Heterogeneity of fracture filling minerals 【Parameters】 <ul style="list-style-type: none">• In-plane heterogeneity in transmissivity of conductive fractures• Transport parameters (flow wetted surface, transport aperture, dispersivity)	(Äspö and others/JNC) 【Conceptual model】 <ul style="list-style-type: none">• Fracture size• Spatial distribution of conductive fractures• Connectivity of conductive fractures• Compartmentalization• Channeling• Fracture intersection• Spatial variability of aforementioned parameters• 3D distribution of gw chemistry• Heterogeneity of fracture filling minerals 【Parameters】 <ul style="list-style-type: none">• In-plane heterogeneity in transmissivity of conductive fractures• Transport parameters (flow wetted surface, transport aperture, dispersivity)		(Äspö and others/JNC) <ul style="list-style-type: none">• TRUE BS : Fracture network of minor fractures less than size of 30m.• TRUE BS:• TRUE-1:Microstructure of fracture including gouge
				【Useful investigation to reduce uncertainty at this stage, Useful multiple lines of evidence】	【Useful investigation to reduce uncertainty at this stage】	【Useful investigation to reduce uncertainty at this stage】	【Useful investigation to reduce uncertainty at this stage】
				(Äspö and others/JNC) <ul style="list-style-type: none">• fluid logging to identify minor conducting features and determining transmissivity• Pressure interference monitoring during drilling. .(II a-2-F2, II a-3-F2)	(II b-F2)	(III-F2)	(IV-F2)
Important issues or lessons learned in constructing GCM	Site Scale	(I-G1)	(II a-1-G1)	(ANDRA) Standard methods of petroleum exploration are effective for characterizing large volumes of sedimentary rock. No significant surprises.	(Äspö and others/JNC) 【Hydrogeology】 <ul style="list-style-type: none">• Uncertainty remains for connectivity of major conductors.• Method to determine representative transmissivity of major conductors. (Is model calibration against response during pumping test only way?) 【Hydrochemistry】 <ul style="list-style-type: none">• 3D spatial distribution of gw chemistry is not understood.• Reconciliation with flow model is important.• Groundwater chemistry data in average rock is rather poor. (II b-G1)	(Äspö and others/JNC) <ul style="list-style-type: none">• gw chemistry change data during tunnel construction provided mainly on the gw chemistry within major conducting features (III-G1)	(IV-G1)
G0							

	Local Scale				<div>Major conductors can be basically understood. However, fractures in average rock are not clear.</div> <div>Poverty in information to construct local scale model.</div> <div>The method to estimate flow wetted surface not established.</div>		<div>【Hydrogeology】</div> <div>Minor structures (ca.<30m) were not detected with TRUE BS borehole array.</div> <div>Channeling structure and fracture intersections are not clear.</div> <div>Internal structure of fracture including gouge and its heterogeneity are not clear.</div>
	G2	(I-G2)	(II a-1-G2)	.(II a-2-G2, II a-3-G2)	(II b-G2)	(III-G2)	(IV-G2)
Numerical models used for PA at this event.	Site scale			<div>(Äspö/JNC)</div> <div>Stochastic continuum model</div> <div>Discrete fracture network model</div> <div>Pipe network model</div> <div>(SKB)</div> <div>During the complete SC phase we are building an integrated description of the site and its regional environments with respect to current state and naturally ongoing processes. Field measurements are analyzed and interpreted for the needs of Design and Safety assessment • <i>Example</i> geology ISI: The site descriptive geological model version 1.2 should include:</div> <div>Description of the geological evolution</div> <div>A geometrical framework and geological parameter values describing the different domains:</div> <div><div>deformations zones (identified based on lineament maps, geological single-hole interpretation, seismic and radar reflections, ...)</div><div>rock domains (identified based on surface geological description, geological single-hole interpretation, ...)</div></div> <div>Parameter description including spatial variability and uncertainty</div> <div>Alternative geometrical framework</div> <div>(ANDRA)</div> <div>Continuum models at scale of Paris Basin and a sector scale model</div> <div>PORFLOW</div> <div>ALLIANCE platform</div>	<div>(Äspö/JNC)</div> <div>Stochastic continuum model</div> <div>Discrete fracture network model</div> <div>Pipe network model</div>		
				<div>(DOE, YMP)</div> <div>Numerical 2D Model</div> <div>-Matrix should be saturated fully before fracture flow</div> <div>-Infiltration/Percolation flux is low</div> <div>-Only matrix flow near repository horizon</div> <div>-Significant lateral flow (~50%)</div> <div>Use of Equivalent Continuum Model</div>	<div>(DOE, YMP)</div> <div>3D Site Model</div> <div>Spatial distribution of infiltration (some areas with high fluxes)</div> <div>Effect of discrete faults</div>		<div>(DOE, YMP)</div> <div>Dual Permeability Model</div> <div>Active Fracture Model</div>
H0	H1						

				<p><i>What level of details are you going to achieve? Why and how do use these models? Ex. Use stochastic continuum to understand site scale flow and to derive BC's for the local scale model. Can you get all parameters from the site? If not, how you assumed and justify the lacking parameters?</i></p>	<p><i>How do use these models? And why?</i></p>		
	Local scale H2			<p>(Äspö/JNC) • Discrete fracture network model • Pipe network model</p> <p>(ANDRA) No local scale model</p> <p><i>What level of details are you going to achieve? Why and how do use these models? Can you get all parameters from the site? If not, how you assumed and justify the lacking parameters? How do you calibrate your model against available data?</i></p>	<p>(Äspö/JNC) • Discrete fracture network model • Pipe network model</p> <p><i>How do use these models? And why?</i></p>		<ul style="list-style-type: none"> • Discrete fracture network model • Pipe network model
Uncertainty in PA models at this event in addition to GCM uncertainties	Site scale			<p>【Uncertainty reduced in event iv】</p>	<p>【Uncertainty reduced in event vi】</p>	<p>【Uncertainty reduced in event viii】</p>	<p>【Uncertainty reduced in event ix】</p>
	I1			<p>(ANDRA) PA at this stage shows that the argillite can contain radioactive waste in the undisturbed scenario. The uncertain isotopes are non-sorbing species like I and Cl.</p> <p>• Describe whether uncertainty in PA model is same with descriptive GCMs. If there is difference, describe reasons and event. => Potential issue could be the long-term aspects (not just understanding the present flow system, but understanding paleohydrology and future hydrogeology.</p>	<p>->same as left</p>		
				<p>【Uncertainty remaining at event iv】</p>	<p>【Uncertainty remaining at event vi】</p>	<p>【Uncertainty remaining at event viii】</p>	<p>【Uncertainty remaining at event ix】</p>

10				<p>(ANDRA)</p> <p>The main uncertainties at this stage come from the impact the EDZ on short-circuit pathways. the retention behaviors of weakly sorbing radionuclides, and the details of the pathway, especially the discharge locations for the encasing units. The current PA is a pessimistic case with upward hydraulic gradients across the host rock. Downward gradients, such as at the lab site, could improve the PA.</p> <p>The scenarios do not take into account the elevated pore pressures of the host rock and its possible implications for osmotic and other non-standard coupled phenomena.</p> <p>The main data improvements identified by PA in Dossier Argile 2001 are:</p> <ul style="list-style-type: none">-Transport and retention properties of argillite host rock- Hydrologic modeling uncertainties:<ul style="list-style-type: none">-refine data for encasing formations-define better the exit points of the flow system-better definition of retention properties for I-29 and CI-36- EDZ taken pessimistically – needs much better characterization and understanding <p>These are addressed in current and future programs</p>	->same as left		
	Local scale			【Uncertainty reduced in event iv】	【Uncertainty reduced in event vi】	【Uncertainty reduced in event viii】	【Uncertainty reduced in event ix】
				<ul style="list-style-type: none">• Describe whether uncertainty in numerical model is same with descriptive GCMs. If there is difference, describe reasons and event (critical measurement).	->same as left		
				【Uncertainty remaining at event iv】	【Uncertainty remaining at event vi】	【Uncertainty remaining at event viii】	【Uncertainty remaining at event ix】
	I2			<ul style="list-style-type: none">• Describe which remaining uncertainty is critical for PA.• Flow wetted surface• Connectivity (Compartmentalization)• Role of EDZ	•		(Äspö/JNC) <ul style="list-style-type: none">• Spatial distribution of conducting fractures (fracture size <30m)• Fracture intersection• In-plane heterogeneity of fracture transmissivity• Micro scale conceptual model of fracture
Event for construction of PA numerical model (when and how the model changed)	Site Scale J1		•	<ul style="list-style-type: none">• Describe whether uncertainty in numerical model is same with descriptive GCMs. If there is difference, describe reasons and event.	•		
J0	Local scale J2			<ul style="list-style-type: none">• Describe whether uncertainty in numerical model is same with descriptive GCMs. If there is difference, describe reasons and event.			(Äspö/JNC) <ul style="list-style-type: none">• Block Scale tracer experiments revealed compartmentalized fracture network system, variability in micro scale conceptual model, and possible fracture intersection effect.

Information used in PA at this event besides in-situ data at the site	Lab. Tests K1				(Äspö/JNC) e.g.) • De, Kd →Data utilized at PA calculation at the final stage of surface based investigation. e.g.) • Dispersion length: 1/10 of travel distance. • Flow wetted surface was estimated from the proportion of conductive fractures. • Matrix diffusion coefficient was measured only for HTO and cations in part. Others were estimated from anion exclusion, surface diffusion. Kd was selected from generic database taking into account of gw chemistry (saline/fresh)		(Äspö/JNC) • Large scale rock block test (ca.50cm) is useful to study in-plane heterogeneity and fracture intersection. • Measuring diffusivity of fracture gouge is important to interpret in-situ tracer experiment.
	Others K2		•	(ANDRA) Data for retention and diffusion are generic and laboratory values at this stage. PA has identified a need for actual in situ data both from the BURE URL and other sources such as Mont Terri	•		
Generic In-situ information (Value of information from other sites including URLs)	L			(Äspö and others/JNC) 【Conceptual model】 • Major conducting features and average rock • Discrete fractures within average rock • Micro scale model inside fracture 【Parameters】 • Dispersion length:1/10 of transport distance • Transport aperture proportional to square root of transmissivity. • Flow wetted surface area: 20-25% of fracture surface area	(ANDRA) Presently for Dossier 2005 the Mont Laboratory is providing very important complementary data on diffusion, EDZ behavior and evolution, and behavior of EDZ cut-offs, among other topics. •Describe the conceptual model/parameters which can be estimated from other sites in case these are not available at the site => such as flow wetted surface area		
Types of feedback from PA to site investigation at this stage.	M	• List up all possible FEPs, prioritize and plan site (SKB) PA (and Design) help us to explain the complexity of the system, to support priorities among development of investigation methods, provide us with analyses that supports the “show stoppers” of site characterization. All that is needed in order to have a well-based site characterization programme.		<div> <div>ii</div> <div>iii</div> <div>iv</div> <div>v</div> </div>	<div> <div>vi</div> <div>Timing of feedback</div> <div>▽</div> </div>		• Block Scale tracer experiment provided the importance of De and Kd of gouge

			(ANDRA) FEPs: Intrusion by water exploration well Well intrudes gallery RISS type glaciation Global warming Maximum possible earthquake Exploitation of deep geothermal resources			
Important issues/lessons learned or recommendation in construction of PA models and feedback. N	(SKB) Interaction between main activities during SC planning of great benefit for improved feedback/communication during actual SC. Comprehensive PA (SR 97) basis for much of our planning and has given also PA model lessons learnt.		(Äspö and others/JNC) • Site scale major conducting features serve to provide BC's to local scale model and to define discharge area for biosphere assessment. • Local scale including EDZ provided most of transport resistance within geosphere. • Hydraulic barrier effect of site scale major conducting features potentially divert the flow upward and provide shorter travel distance. (SKB) Keep in mind the Swedish experience of site specific safety assessments for three sites in Sweden (SR 97) and of site investigation and evaluation at Äspö. All this has already affected the PA approach, models and means of feedback and also affected the SC programme as well as organization. Our best contribution here could perhaps be to tell the story of SKB working procedure. On-going site characterization work has not yet provided much additional lessons learnt in this respect. (ANDRA) PA has inspired activities of FSP (deep scientific boreholes) and FRF (fracture characterization boreholes). Feedback will come in preparations for Dossier 2005 report	• Do NOT simply describe the previous experience, but describe how you can make improvement in constructing defensible and reliable PA model and in feedback from PA to site characterization.		

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