SKI Report 00:47

Opinions on SKB's Safety Assessments SR 97 and SFL 3-5

A Review by SKI Consultants

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Foreword

The Swedish Nuclear Fuel and Waste Management Co. (SKB) has presented their safety assessment ”Deep repository for spent nuclear fuel, SR 97 – Post-closure safety”. SKB’s report is part of the documentation that has been required by the Government before the start of site investigations.

The Swedish Nuclear Power Inspectorate (SKI) is reviewing SR 97 according to earlier Government decisions. In its review work SKI has asked several consultants, that recently have been performing research work for SKI, to give their opinions on SR 97. SKI and the Swedish Radiation Protection Institute (SSI) have used these reports from the consultants as one complementary basis for the formulation of the SKI/SSI review report (SKI Report 00:39; SSI Report 2000:17).

This is a compilation of the reports from the different consultants, and therefore the different contributions vary in length, style and language.

Included are also two consultant reports, giving comments on SKB’s preliminary safety assessment for SFL 3-5 (deep repository for long-lived low- and intermediate-level waste).

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Randolph C. Arthur
Wei Zhou

Monitor Scientific, LLC
3900 S. Wadsworth Blvd., Suite 555
Denver, Colorado 80235, USA

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Executive Summary

The Swedish Government has asked SKB to carry out a safety assessment of the KBS-3 disposal concept for spent nuclear fuel "…to demonstrate that the KBS-3 method has good prospects of being able to meet the safety and radiation protection requirements which SKI and SSI have specified in recent years." The results of that assessment, referred to as SR 97, have recently been published. The present report summarizes the results of a review of selected geochemical aspects of SR 97. These subjects include the hydrochemical evolution of a defective canister, thermodynamic data supporting estimates of radioelement solubilities, modeling of near-field chemistry and analyses of the effects of ice melting on propagation of an oxidizing front to repository depths.

The primary focus of the review is on the canister-defect scenario, and, more specifically, on supporting analyses of the hydromechanical evolution of a defective canister. The results of these analyses figure prominently in the safety assessment because they suggest that even a defective canister will, in effect, remain dry for as long as 200,000 years. This is an important constraint because it is taken in SR 97 as the period of time required for a continuous water pathway to form in the near field. The transport of most radionuclides (*i.e.*, those that do not exist as a gas) cannot occur until this pathway is formed.

It is concluded that although SKB's hydromechanical models are sound, they may suffer from an over-simplification of the chemical processes involved. Analyses using the models do not acknowledge that the chemical system within the canister is open in all respects to the chemical system in the buffer. Instead, mass transfer across the defect at the canister-buffer interface is limited to liquid H_2O and water vapor. Consideration of mass transfer of other gases [*e.g.*, $CO_2(g)$ and $H_2S(g)$] dissolved in buffer porewaters suggests that associated reactions involving the iron insert and inner surfaces of the copper shell may stabilize corrosion products (e.g., siderite, pyrite, Cu sulfides) that are not presently considered in SKB's models. The effects on the hydrochemical evolution of the canister resulting from the progressive concentration of solutions as H_2O is consumed by corrosion of the iron insert is also not considered in SKB's models. The assumption in these models that iron corrodes in contact with water vapor is also questionable. Experimental evidence cited in support of this assumption suggests that in fact a condensation step is first required. If so, then a condensation mechanism [*e.g.*, capillary condensation (?)], under relevant thermal conditions expected in the near field, should be proposed and backed up with experimental evidence. If not, then a credible mechanism for corrosion of the insert in the presence of gaseous H_2O should be elucidated on the basis of experimental investigation.

The internal consistency of the thermodynamic database used in SR 97 to estimate radioelement solubilities is not evaluated by SKB. The internal consistency may be poor, however, because selection of preferred values is made with little regard to requirements that must be met, or approximated as closely as possible, to ensure internal consistency. If the database is not internally consistent, then it is difficult to make any objective assessment of its reliability.

The chemistry of the near field is relatively unimportant in SR 97 compared with other international performance assessments, where in particular solubility-limiting constraints on the source term are based on predictions of the long-term chemical evolution of buffer porewaters. The rationale for this latter approach is that the properties of bentonite-porewater systems are thought to be better characterized and more likely to be time invariant than corresponding properties of other engineered barrier components or the geosphere. SKB have apparently rejected this line of reasoning, and, if so, an explanation supporting this decision would be helpful.

The chemical evolution of buffer porewaters resulting from the interaction of MX-80 bentonite with Äspö, Finnsjön or Gideå groundwaters has been modeled by SKB. The results are not used in SR 97, however. Rather, a modeled porewater composition resulting from the interaction of MX-80 bentonite with a synthetic, Allard-type groundwater is used to estimate near-field radioelement solubilities. If these solubilities are greater than those calculated for the Äspö, Finnsjön or Gideå groundwaters, then the near-field solubilities are conservatively used in SR 97. There is no explanation, however, why the apparently more relevant buffer models (*i.e.*, those based on interactions with Äspö, Finnsjön or Gideå groundwaters, rather than a synthetic groundwater) were not used to estimate near-field solubilities in SR 97. It is also noted that despite previous questions from SKI concerning SKB's approach to modeling bentonite-water interactions, these questions are not addressed in SKB's more recent modeling studies.

The potential for oxygenated solutions resulting from the melting of an ice sheet to migrate to repository depths is mentioned in several places in the summary and main reports documenting SR 97. A modeling study commissioned by SKB basically confirms earlier analyses by SKI indicating that this scenario is possible, although unlikely. It is important to bear in mind that this conclusion is based on scoping calculations using simplified models of complex hydrochemical-hydrogeologic processes driven by a climate-change scenario. For this reason, SKI's earlier recommendation that SKB should examine the geologic record for any indications of past migration of oxygenated solutions to the deep subsurface is still reasonable.

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1 Defective-Canister Scenario

The canister-defect scenario considered by SKB in SR 97 involves an analysis of the hydromechanical evolution of a defective canister. The analysis is described by Bond *et al.* (1997). The main results are confirmed in an independent study by Takase *et al.* (1999). The results from both studies figure prominently in SR 97 because they suggest that even a defective canister will remain essentially dry for as long as 200,000 years. This is an important constraint in the canister-defect scenario because it is taken as the period of time required for a continuous water pathway to form in the near field (SKB 1999a). The outward transport of most radionuclides (*i.e.,* those that do not exist as a gas) cannot occur until this pathway is formed.

Bond *et al.* (1997) and Takase *et al.* (1999) assume that the canister's cast-iron insert reacts with any porewater entering the canister from the buffer, or with a gas phase saturated with water vapor, according to the following reaction:

$$3Fe + 4H_2O \rightarrow Fe_3O_4 \text{ (magnetite)} + 4H_2, \qquad (1)$$

for which the corresponding equilibrium partial pressure of hydrogen is approximately 1000 bars. The insert therefore dissolves continuously and irreversibly because the total internal pressure within the canister is always less than or equal to the sum of the hydrostatic pressure (50 bars) and swelling pressure of the buffer (50 bars), and because the insert is assumed to be always in contact with liquid or gaseous H_2O. The corrosion rate is apparently limited by the transport rate of H_2O through a layer of magnetite that adheres to the surface of the insert. The rate is assumed to be in the range 0.01 to 1 $\mu m\ yr^{-1}$, based on experimental measurements reported by Blackwood *et al.* (1994), and is assumed to be constant over the entire period of time considered in the hydromechanical analyses ($\approx 10^5$ yr). Bond *et al.* (1997) stress that this assumption is questionable because the available experimental data only extend over a period of 500 days. Natural analogs that could be used to help better define the long-term corrosion rate exist in the form of natural iron occurrences, extraterrestrial occurrences (*i.e.,* meteorites) and archaeological artifacts (Johnson and Francis, 1980; Miller *et al.,* 1994), but the relevance of these analogs may be questionable because their alloying components are significantly different than those of the carbon-steel inner canister (Johnson and Francis, 1980).

Chemical constraints on the hydromechanical evolution of a defective canister, other than that imposed by reaction (1), are not considered by Bond *et al.* (1997) or Takase *et al.* (1999). These authors therefore assume that the chemical environment in a defective canister is sufficiently similar to experimental systems in which the corrosion behavior of carbon steel has been measured (Blackwood *et al.,* 1994) that the experimental results can be used in the hydromechanical models without modification.

This view may be overly simplistic. Other constraints imposed by reversible and irreversible mass transfer among liquid and gas phases within the canister, and between the canister and buffer, are certainly possible given the inherently open nature of the near field system resulting from the defect in the copper shell. These additional constraints are described in the following section, and evaluated in a preliminary manner to determine how

they might affect some of the assumptions adopted in the hydromechanical models. Comments based on this survey are summarized in Section 1.1.7.

1.1 Survey of processes controlling the chemical environment inside a defective canister

The discussion in this section focuses on the region of the 2 mm annular gap between the outer copper shell and inner iron insert. The presence of a circumferential crack penetrating the insert is ignored because the crack itself would not involve processes different than those considered below. A conceptual model of chemical and transport processes occurring in this region is illustrated schematically in Fig. 1a, where it is assumed that porewater from the buffer has partially filled the gap, and in Fig. 1b, where it is assumed that liquid water no longer exists in the annulus. In Fig. 1a it is assumed that porewater from the buffer flows into the gap as long as the internal pressure in the canister is less than the hydrostatic pressure. This situation approximates the "Assessment Model" described by Bond *et al.* (1997). In Fig. 1b it is assumed that the internal pressure and hydrostatic pressure are equal, and that any water previously entering the canister has been consumed by corrosion of the iron insert. This situation corresponds to the "Diffusion Model" evaluated by Bond *et al.* (1997). A through-going defect penetrating the thickness of the copper shell is assumed to exist. The chemical system in the annulus is therefore open with respect to the chemical system in the buffer. This is a critical difference between the model system depicted in the figures and the barometric cell used to measure the corrosion rate of iron (Blackwood *et al.,* 1994). The experimental system is a closed system.

The chemical and transport processes illustrated in Figs. 1a and 1b are identified by numbered lines terminating in a single arrow (irreversible processes) or double arrows (reversible processes). These processes are discussed below in numerical order.

1.1.1 Corrosion of the iron insert by $H_2O(l)$ – (1)

SKB assume that this occurs in two stages. The first involves initial formation of an adherent inner film of magnetite by an "electrochemical mechanism", which is not described (Blackwood *et al.*, 1994). The inner film provides most of the corrosion protection, and transport through the film is thought to be rate limiting (SKB, 1999b). The corrosion reaction is represented by:

$$3Fe + 4H_2O(l) \rightarrow Fe_3O_4 + 4H_2 \ .$$

Platts *et al.* (1994) review mechanisms that have been proposed for this and similar reactions [*e.g.*, reactions involving formation of $Fe(OH)_2$ rather than magnetite]. The presence of liquid water is apparently required to produce the inner corrosion-product film. Its unclear, however, whether associated reaction mechanisms are equivalent to the electrochemical mechanism invoked by Blackwood *et al.* (1994), who note that formation of the inner film does not involve "going through a Fe^{2+} intermediate stage".

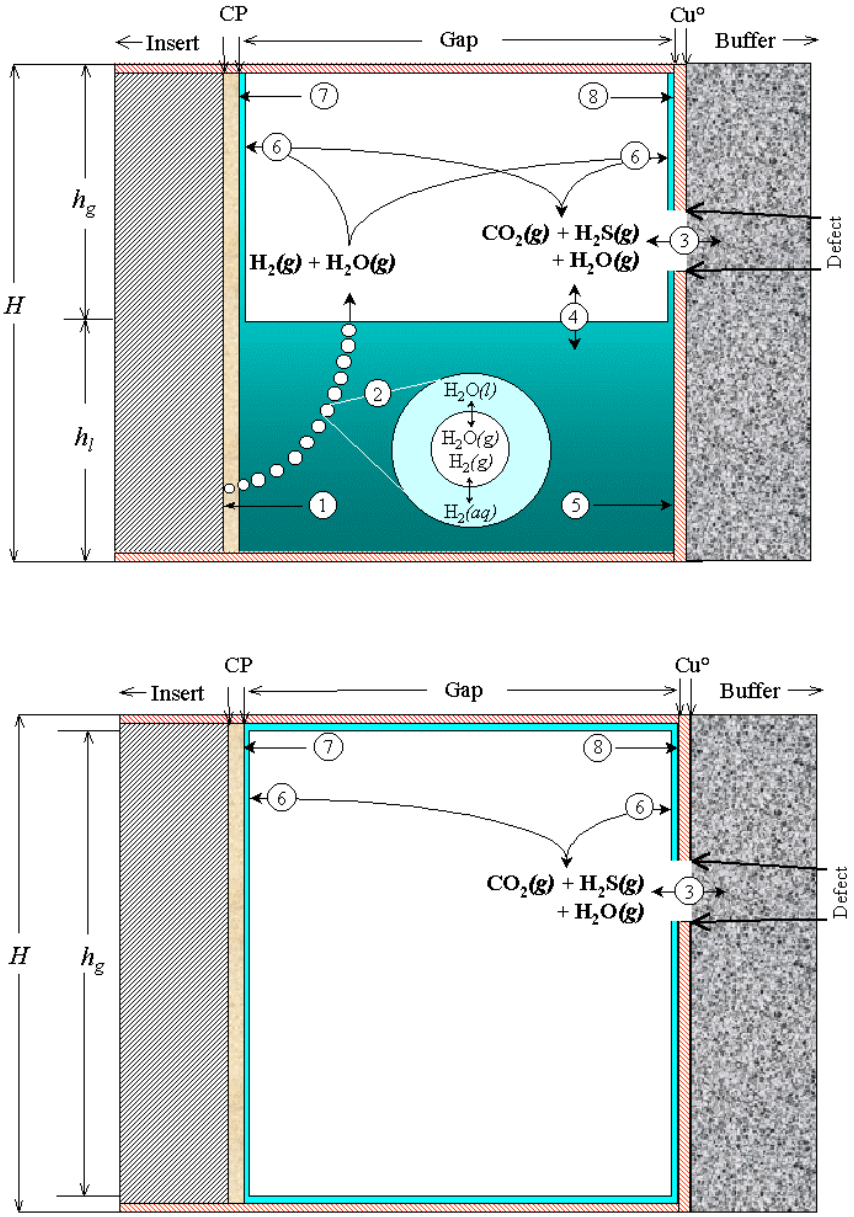

Figure 1. Schematic diagram of chemical and transport processes in the region of the annular gap considered in the canister-defect assessment model (Fig. 1a, top) and diffusion model (Fig. 1b, bottom) of Bond et al. (1997). The processes are indicated by numbers and are discussed in the text. "CP" refers to corrosion products of the iron insert, H denotes the total height of the canister (447 cm), h_l represents the level of the liquid phase and h_g stands for the level of the gas phase.

An outer non-adherent layer of magnetite then forms on the inner film by a precipitation process (SKB 1999b):

$Fe + H_2O(l) \rightarrow Fe^{2+} + H_2 + 2OH^-$

$3Fe^{2+} + 2OH^- + 2H_2O(l) \rightarrow Fe_3O_4 + 3H_2$

[note that the latter reaction is not charge balanced, *i.e.*, the structural formula for magnetite is $(2Fe^{3+}Fe^{2+})O_4$]. Although these reactions involve Fe^{2+}, the corrosion rate does not depend on its concentration because the reaction forming the inner layer is believed to be rate limiting (Blackwood *et al.*, 1994).

1.1.2 Mass transfer of H_2 from liquid to gas - (2)

SKB assume that all the hydrogen produced by corrosion in the liquid phase is transferred to the gas phase. This is inferred from the following aspects of their model (Bond *et al.*, 1997).

Distribution of H_2 between liquid and gas phases. For the conditions considered in Fig. 1a (*i.e.*, no circumferential crack in the insert, and assuming the internal pressure is less than the sum of the hydrostatic pressure and swelling pressure, such that no gas escapes from the canister), the hydrogen production rate is given by (Bond *et al.*, 1997; Appendix A):

$$\frac{dn_i}{dt} = \gamma m_H A_w , \qquad (2)$$

where n_i denotes the number of moles of hydrogen (in the gas phase –see below), t stands for time (yr), γ refers to a dimensionless "corrosion-rate reduction factor", which is equal to unity as long as liquid water exists in the gap, m_H represents the rate at which hydrogen is produced by the corrosion reaction (mol cm^{-2} yr^{-1}), and A_w refers to an "enhanced" area of the corroding surface (cm^2). The hydrogen production rate is related to the corrosion rate by:

$$m_H = m\frac{\sigma_H}{V_{Fe}} , \qquad (3)$$

where m stands for the corrosion rate (cm^3 cm^{-2} yr^{-1}), σ_H = 4/3 refers to the stoichiometric ratio of hydrogen with respect to iron in the corrosion reaction (1), and V_{Fe} represents the molar volume of iron (cm^3 mol^{-1}). The enhanced area of the corroding surface is given by:

$$A_w = A + 2\pi r_c(\alpha - 1)h_l , \qquad (4)$$

where A, defined below, refers to the area of the corroding surface, r_c denotes the radius of the cast-iron insert (47.3 cm), α stands for a dimensionless galvanic enhancement factor, and h_l (cm) stands for the depth of liquid water in the gap (Fig. 1a). Ignoring for the sake

of simplicity the term describing galvanic enhancement of the corrosion rate (*i.e.,* assuming $\alpha = 1$), $A_w = A$, which is given by:

$$A = 2\pi r_c H \,, \tag{5}$$

where H (447 cm) denotes the height of the annulus (Fig. 1a).

The parameter n_i in Eqn. (2) refers to the number of moles of H_2 gas because it is used by Bond *et al.* (1997) to calculate the internal pressure, P_i (bar), given by the ideal gas law:

$$P_i = \frac{n_i RT}{V_{Hi}} \,, \tag{6}$$

where R stands for the gas constant (cm^3 bar deg^{-1} mol^{-1}), T denotes temperature (K) and V_{Hi} refers to the volume of hydrogen in the gas phase (*i.e.,* the volume occupied neither by water nor corrosion products).

An identical rate constant, m, is assumed for the corrosion reaction in both the liquid and gas phases (Bond *et al.,* 1997). The change in number of moles of H_2*(g)* is therefore proportional to the product of the corrosion rate and the total area of the corroding surface [Eqn. (2)]. This implies that the hydrogen produced by corrosion in the liquid phase as H_2*(aq)* is exactly balanced by an equivalent amount lost to the gas phase as H_2*(g)*.

Constraints on redox potentials and corrosion-product mineralogy. If the above interpretation of the distribution of H_2 between liquid and gas phases is correct, then associated constraints on the redox potential of the aqueous phase can be deduced from an analysis of H_2 mass transfer between these phases. This analysis is summarized below.

The loss of an amount of H_2 from the liquid phase that is equivalent to the amount of H_2 produced in that phase by corrosion of the iron insert requires:

$$\frac{dn_{H_2(aq)}}{dt} = \frac{dn_{H_2(aq),c}}{dt} - \frac{dn_{H_2(aq),g}}{dt} = 0 \,, \tag{7}$$

where the first term on the right-hand side of the first identity refers to the production rate of H_2*(aq)* by corrosion and the second term stands for its rate of mass-transfer to the gas phase. Both terms depend on the corrosion rate. The first term is given by (Bond *et al.*, 1997):

$$\frac{dn_{H_2(aq),c}}{dt} = \frac{2\pi r_c m \sigma_H h_l}{V_{Fe}} \,, \tag{8}$$

where $n_{H2(aq)}$ stands for the number of moles of dissolved hydrogen, h_l refers to the height of the liquid phase in the annulus (Fig. 1a) and other parameters are as defined above.

The second term can be evaluated by noting that the hydrogen production rate in the gas phase is equal and opposite to the rate at which water vapor is consumed (Bond *et al.*, 1997):

$$\frac{dn_{H_2O}}{dt} = -\frac{dn_{H_2(g)}}{dt} = -\frac{2\pi r_c m \sigma_H h_g}{V_{Fe}}, \tag{9}$$

where h_g refers to the height of the gas phase in the annulus (Fig. 1a). Bond *et al.* (1997) demonstrate that the transport of water vapor within the canister is practically instantaneous in comparison with the growth rate of magnetite on corroding surfaces. This implies that the gas phase is continuously saturated with water vapor. The amount of vapor consumed by the corrosion reaction must therefore be balanced by evaporation of an equivalent amount of H_2O from the liquid phase (assuming negligible evaporation of water from pores in the buffer). The evaporation rate is thus equal but opposite in sign to the rate at which water vapor is consumed by the corrosion reaction:

$$\frac{dn_{H_2O,e}}{dt} = \frac{2\pi r_c m \sigma_H h_g}{V_{Fe}}, \tag{10}$$

where $dn_{H2O,e}$ refers to the number of moles of H_2O evaporated.

The new volume of gas created by evaporation must equilibrate with H_2 dissolved in the liquid phase in accordance with Henry's Law. This process is shown in Fig. 1a, where it is assumed for illustration purposes that evaporation involves formation of a bubble. A convenient expression for the equilibrium distribution of H_2 between liquid and gas is given by (Drummond and Ohmoto, 1985; Arthur and Murphy, 1989):

$$\kappa_{H_2} = \frac{m_{H_2(g)}}{m_{H_2(aq)}}, \tag{11}$$

where κ_{H2} stands for the dimensionless "volatility ratio", $m_{H2(g)}$ represents the molality of $H_2(g)$ (*i.e.*, per kilogram water vapor) and $m_{H2(aq)}$ refers to the molality of $H_2(aq)$[1]. The rate at which H_2 is transferred from the liquid phase by evaporation of H_2O is then given by:

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[1] The volatility ratio is related to the Henry's Law constant by (Drummond and Ohmoto, 1985):

$$\kappa_{H_2} = \frac{\omega K_{H,H_2} \gamma_{H_2(aq)}}{\rho_g \phi_{H_2(g)} ZRT},$$

where ω represents a conversion factor equal to 1000 g kg^{-1}, K_H stands for the Henry's Law constant, $\gamma_{H2(aq)}$ denotes the activity coefficient of $H_2(aq)$, ρ_g refers to the density of water vapor (g cm^{-3}), $\phi_{H2(g)}$ represents the fugacity coefficient and Z stands for the compressibility factor.

$$\frac{dn_{H_2(aq),g}}{dt} = m_{H_2(g)}\frac{dW_{H_2O}}{dt} = \frac{\kappa_{H_2} m_{H_2(aq)} \mathrm{M}_{H_2O}}{1000}\frac{dn_{H_2O,e}}{dt}$$

$$= \frac{2\pi r_c m \sigma_H h_g \kappa_{H_2} m_{H_2(aq)} \mathrm{M}_{H_2O}}{1000 V_{Fe}} \qquad (12)$$

where W_{H2O} and M_{H2O} stand for the mass (g) and molecular weight (g mol^{-1}) of H_2O, respectively, and the factor 1000 refers to the number of grams in one kilogram.

Substituting Eqn. (8) and the final identity of Eqn. (12) into Eqn. (7) leads to the following expression:

$$m_{H_2(aq)} = \frac{1000}{\kappa_{H_2} \mathrm{M}_{H_2O}}\frac{h_l}{h_g}. \qquad (13)$$

At 25°C and the range of pressures considered in the hydromechanical model, the volatility ratio for H_2 is essentially constant and equal to 1.2 x 10^6 (Drummond, 1981), indicating that H_2 is strongly partitioned to the gas phase in evaporating systems. It is important to note that κ_{H2} does, however, increase rapidly with increasing ionic strength. The molecular weight of H_2O is also a constant equal to approximately 18 g mol^{-1}. Variations in the molality of H_2*(aq)* under conditions where the ionic strength is relatively low (*e.g.*, less than about 1 molal) are therefore a function of the height of the liquid phase within the gap, given by:

$$m_{H_2(aq)} = 4.6\text{x}10^{-5}\frac{h_l}{H - h_l}. \qquad (14)$$

A plot of this function is shown in Fig. 2, where it can be seen that the aqueous molality of H_2 should lie roughly in the range 10^{-9} to 2 molal for liquid levels in the annulus between 0.01 to 446 cm, respectively. Extrapolation of this function to the condition $h_l = H$ is inappropriate because evaporation is then no longer possible. Similarly, there must be a lower limit to h_l, possibly on the order of a few molecular diameters thick, below which H_2O ceases to exist as a discrete liquid phase.

The stability of minerals in the system FeO-Fe_2O_3-H_2O is shown in Fig. 3 as a function of pH over the range of H_2*(aq)* concentrations plotted in Fig. 2. As can be seen, magnetite is stable over most of the range of possible H_2*(aq)* molalities that could exist in the annulus, except when $m_{H2(aq)}$ is less than about $10^{-8.6}$ mol kg^{-1}. This corresponds to liquid levels in the annulus less than about 0.1 cm (see Fig. 2).

Hematite is predicted to be stable if $m_{H2(aq)}$ is less than about $10^{-8.6}$ mol kg^{-1}. Hematite is kinetically inhibited from precipitating from aqueous solutions at low temperatures, however, and it is therefore likely that a metastable solid such as goethite would form in its place. If so, the lower limit of magnetite stability is shifted to lower values of $m_{H2(aq)}$ (e.g., about 10^{-12} mol kg^{-1} for the case of goethite), and thus to smaller values of h_l.

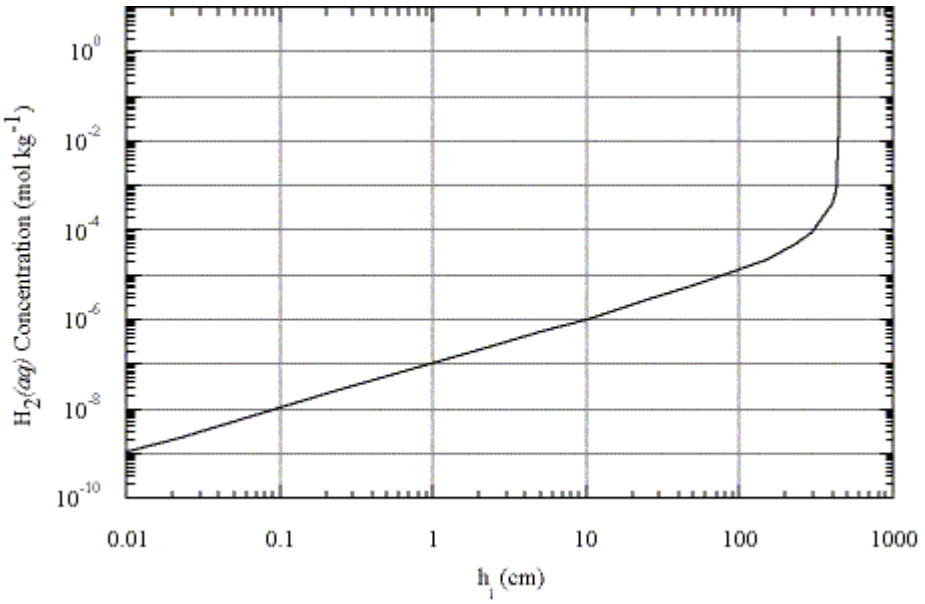

Figure 2. Concentration of $H_2(aq)$ as a function of the liquid level (h_l) in the annulus.

Figure 3 is drawn assuming an arbitrary aqueous concentration of Fe^{2+} equal to about 10^{-5} mol kg^{-1}. Variations in the concentration of Fe^{2+} shift the nearly vertical mineral-solution equilibrium boundaries to the left or right, however, and do not affect the stabilities of magnetite and hematite relative to the molality of $H_2(aq)$ (indicated by the horizontal line).

It is also important to note that minerals other than corrosion products may precipitate in the annulus when water ceases to flow into the gap and corrosion advances to a stage that most of the water initially present is converted to $H_2(g)$. Preliminary calculations indicate that when after roughly 95% of the H_2O is consumed by the corrosion reaction, an increasingly saline residual solution is generated (ionic strengths exceeding 6 molal) and that a variety of salts and ferrous aluminosilicate minerals precipitate. The types and amounts of minerals precipitated depends on the amount of solution present in the gap when flow ceases and the solution's initial composition.

Based on the results depicted in Figs. 2 and 3, the assumption adopted in the hydromechanical models that magnetite is the stable corrosion product of iron appears to be reasonable, except possibly at very low levels of the liquid phase in the annulus. It may be unrealistic to assume that hematite could precipitate under these conditions, however, in which case magnetite would probably be the stable corrosion product over the full range of possible liquid levels in the gap. This conclusion is based, however, on the assumption that mass transfer of gases from the buffer into the region of the annular gap does not occur. This possibility is considered in the following section.

1.1.3 Gas-liquid equilibria - (3) & (4)

If transport in the gas phase within the annulus is rapid, as demonstrated by Bond *et al.* (1997), it is reasonable to assume that this phase will equilibrate with volatile aqueous species dissolved in the buffer's porewater according to Henry's Law. In addition to H_2O,

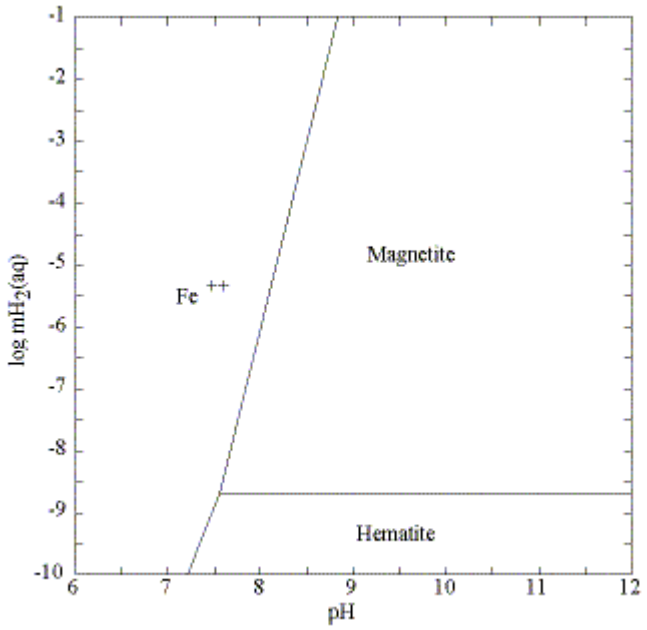

Figure 3. Stability relations among minerals in the FeO-Fe_2O_3-H_2O system at 25ºC (log a_{Fe2+} = -4.8).

these species include CO_2*(aq)* and H_2S*(aq).* The composition of the gas phase will therefore include H_2O*(g),* CO_2*(g)* and H_2S*(g).* Gas species entering the gas phase from the buffer may also equilibrate with the liquid phase in the annulus (Fig. 1a) and any condensate (see below) forming on the surface of the iron insert and copper shell (Figs. 1a and 1b). Mass transfer of volatile species across the buffer porewater-gas interface will be controlled in part by the rate of diffusion of these species from the interior of the buffer to the interface. The concentrations of CO_2*(aq)* and H_2S*(aq)* in buffer porewaters are likely to be controlled by mineral-fluid reactions, but not by oxidation-reduction equilibria (*i.e.*, these reactions are too slow unless they are catalyzed by microbiological activity, or possibly by contact with metal surfaces in the canister).

Should the liquid phase in the annulus equilibrate with CO_2*(g)* and H_2S*(g)* derived from the buffer, the relative stabilities of corrosion products of the iron insert are significantly altered compared with conditions shown in Fig. 3. A figure analogous to Fig. 3 is shown in Fig. 4, where it is assumed that the partial pressures of CO_2*(g)* and H_2S*(g)* are fixed by solubility equilibrium at $10^{-3.5}$ and $10^{-7.8}$ bars, respectively. Carbon dioxide partial pressures in deep groundwaters range roughly from 10^{-3} to 10^{-6} bars, and the value selected here is therefore near the upper bound of this range. The selected partial pressure of H_2S*(g)* is calculated based on Henry's law assuming a total dissolved S(II) concentration of 0.5 mg/kg, and assuming that all the sulfide is in the form of H_2S*(aq).* The assumed concentration lies within the range of sulfide concentrations (0.1 – 1 mg/kg) observed in Swedish groundwaters and bentonite-water interaction tests (Hermansson and Eriksson, 1999). The corresponding partial pressure represents a maximum value, however, because all the dissolved sulfide is assumed to be in the form of H_2S*(aq).*

As can be seen in Fig. 4, the stability range of magnetite with respect to $m_{H2(aq)}$ (and thus h_l, see Fig. 2) is significantly reduced compared with that shown in Fig. 3, and is bounded by the stability fields of siderite ($FeCO_3$) and pyrite (FeS_2). Both these minerals are known to

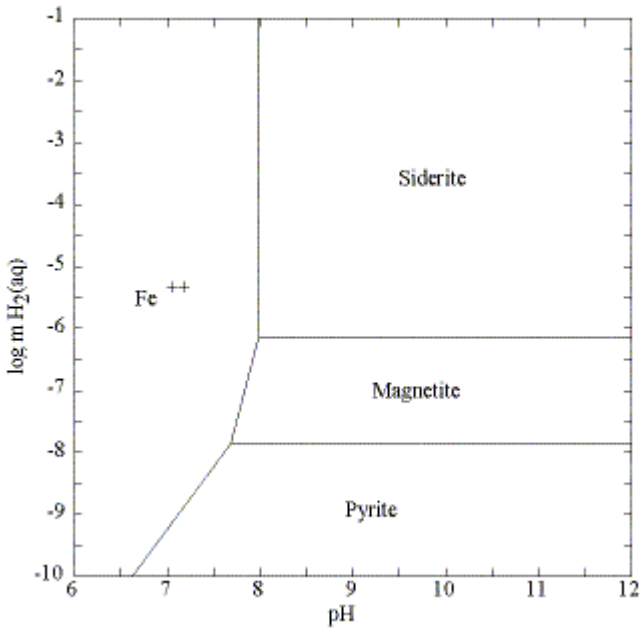

Figure 4. Stability relations among minerals in the FeO-Fe_2O_3-CO_2-H_2S-H_2O system at 25ºC (log a_{Fe2+} = -4.8; log $f_{CO2(g)}$ = -3.5; log $f_{H2S(g)}$ = -7.8).

precipitate relatively rapidly at low temperatures, and their existence as stable corrosion products of iron must therefore be assumed if liquid levels in the annulus are in the appropriate range. As can be inferred from Figs. 4 and 2, corrosion of the insert to form magnetite can only occur if the liquid phase in the gap rises to a height between about 0.1 and 10 cm. The relative stability of magnetite increases at the expense of siderite when $P_{CO2(g)}$ decreases. It increases at the expense of pyrite when $P_{H2S(g)}$ decreases. Because maximal partial pressures of both these gases are assumed, the consequent shrinkage of the magnetite stability field relative to that shown in Fig. 3 probably represents the maximum possible extent under repository-relevant conditions.

The assumption adopted in the hydromechanical model that magnetite is the only stable corrosion product of iron is thus open to question. Magnetite, siderite and/or pyrite may be stable depending on the molality of $H_2(aq)$ and the partial pressures of $CO_2(g)$ and $H_2S(g)$. The chemistry of porewater in the buffer, and possibly of groundwater in the nearby host rock, and mass-transport and mass-transfer processes near the porewater-gas interface must be taken into account before reliable predictions can be made concerning which of these phases is the stable corrosion product of iron.

1.1.4 Corrosion of the copper shell – (5)

Based on the preceding discussion, it is reasonable to assume that the liquid phase in the gap will contain dissolved sulfide. If so, the interior surface of the copper shell will be subject to corrosion and formation of copper sulfide corrosion products. The overall corrosion rate of the shell would thus increase in proportion to the surface area contacted by the liquid phase in the annulus.

1.1.5 Condensation and equilibration of the condensate with $CO_2(g)$ and $H_2S(g)$ – (6)

It is assumed in the hydromechanical models (Bond *et al.*, 1997 and Takase *et al.*, 1999) that the cast iron insert corrodes in contact with water vapor according to reaction (1). This assumption is based on experimental results described by Blackwood *et al.* (1994), who observed that carbon steel wires suspended completely clear of a reservoir of artificial groundwater in a humid atmosphere corroded at the same rate as wires immersed in water. Differences were observed, however, in the initial hydrogen production rates and in the time required to form the protective magnetite layer. These differences are attributed to condensation of water vapor on surfaces of the suspended wires. The condensate would be more dilute and hence more acidic than solutions in which the wires were completely immersed, and the lower pH may therefore have accelerated the corrosion rate (Blackwood *et al.*, 1994).

The presumption that iron corrodes in contact with water vapor may therefore be questionable. It appears from the experimental results noted above that in fact water vapor must first condense before corrosion can occur. Neretnieks (1985), citing personal communications from R. Grauer and E. Mattsson as the only supporting evidence, also concludes that iron will not corrode unless it is in contact with liquid water. This may conflict with the view held by SKB, however, who note that the inner adherent layer of magnetite that has been observed on fresh iron surfaces forms by an "electrochemical mechanism" (Blackwood *et al.*, 1994). If so, it would be helpful if SKB can explain what this mechanism actually entails.

If iron corrosion in the gas phase requires condensation of water vapor, then the question arises whether a suitable mechanism exists for condensation to occur under conditions considered in the hydromechanical models. For example, a slight temperature gradient between the insert and the buffer is in the wrong direction for water to condense on the surface of the insert. If a realistic mechanism for condensation does not exist, then the scenario of pressure build up and hydrogen release must be controlled entirely by the rate of corrosion in the liquid phase. Unless the liquid phase completely fills the gap, this rate will be lower, possibly much lower, than the rate considered in the hydromechanical models.

Water vapor may condense in isothermal porous media by the process of capillary condensation. The equilibrium vapor pressure over a curved surface is less than that over a planar surface due to the change in free energy required to sustain the curvature. The reduction in vapor pressure is related to the radius of a circular pore by the Kelvin equation (*e.g.*, Adamson, 1967; p. 58):

$$\ln\left(P_{H_2O}\big/P^0_{H_2O}\right) = -\frac{2\Gamma V}{r_p RT}, \qquad (15)$$

where P_{H2O} stands for the vapor pressure (bar) in a pore of radius r_p (cm), P^0_{H2O} refers to the corresponding pressure over a planar surface, Γ denotes the surface tension of the solution (dynes cm^{-1}) and V represents its molar volume (cm^3 mol^{-1}). On the basis of this equation, it is reasonable to assume that a gas phase saturated with water vapor in contact

with a planar surface will condense if the gas migrates into a porous medium where the pore size is sufficiently small. This possibility is discussed in the context of a steel canister in direct contact with a bentonite buffer by Neretnieks (1985).

Here we apply similar reasoning to conditions considered in the Assessment Model (Fig 1a) and Diffusion Model (Fig. 1b) described by Bond *et al.* (1997). In the Assessment Model it is assumed that a liquid phase exists in the annular gap. If the corrosion-product layer is assumed to be porous, then water will condense in the pores if the pore size is less than the width of the gap (a maximum of 2 mm). Although this seems likely, it depends on the physical structure of the corrosion-product layer, for which direct experimental data are apparently lacking. In the Diffusion Model a liquid phase does not exist in the gap. Capillary condensation will then depend on the relative size of the pores in the corrosion-product layer compared with the size(s) of pores in the buffer. If the latter are smaller than those of the corrosion-product layer, then liquid water will not condense in the corrosion-product layer. This is possible, if not likely (Neretnieks, 1985), and if so corrosion of the iron insert will not occur.

If it is simply assumed that a suitable mechanism exists whereby water vapor is able to condense within the pores of corrosion products, the resultant liquid phase would be expected to equilibrate with $CO_2(g)$ and $H_2S(g)$ in the coexisting gas phase. Both these gases form weak acids when dissolved in aqueous solution. For example, the pH of a dilute solution equilibrated with a gas in which $P_{CO2(g)} = 10^{-3.5}$ bar is 5.6. The condensate, if it forms at all, will therefore be dilute and mildly acidic.

1.1.6 Reaction of corrosion products with condensate – (7) & (8)

Based on the preceding discussion, it is possible that water vapor will condense within pores of the corrosion products formed on the surface of the iron insert, and possibly on the inner surface of the copper shell. Equilibration of the condensate with $CO_2(g)$ and $H_2S(g)$ in the coexisting gas phase, which is also equilibrated with buffer porewater, would make the condensate mildly acidic. Magnetite and siderite are stable at low Fe^{2+} concentrations in alkaline solutions, but may not be stable in acidic solutions unless the concentration of Fe^{2+} also increases significantly. Thus if liquid water exists in the annulus (Assessment Model; Fig. 1a) the stable corrosion products of the insert may differ depending on whether corrosion takes place in the presence of the liquid or gas phase.

1.1.7 Comment summary

The otherwise excellent analyses by Bond *et al.* (1997) and Takase *et al.* (1999) supporting SKB's contention in SR 97 that even a defective canister would remain effectively dry for as long as 200,000 years suffer from an oversimplification of the chemical processes involved. The analyses do not acknowledge that the chemical system within the canister is open in all respects with the buffer's system. Instead, mass transfer across the defect at the canister-buffer interface is limited to liquid H_2O and water vapor. Takase *et al.* (1999) consider the possibility that a gel-like phase from the buffer could flow, or extrude, into the annular gap in the canister, but they only evaluate physical consequences on the ability of this material to later imbibe porewater from the buffer.

Despite this criticism, the question remains whether alternative models that include one or more of the chemical processes discussed above would invalidate the main contention that the canisters remain dry for long periods of time. The key question here seems to be whether iron can corrode in contact with water vapor, or whether a condensation step is required. If it can corrode in contact with water vapor, then SKB should be more forthcoming in explaining this mechanism and its rate. If condensation is necessary, then the question is how, and where, does this occur – on the metal's surface or farther away in the corrosion product layer? If condensation occurs in the corrosion-product layer, then how does it "flow" from there to the metal's surface (and at what rate)? Would the magnetite (and/or siderite or pyrite), be stable in contact with the resultant acidic solution? Finally, it would be worthwhile to examine more closely the possibility that the inner surface of the copper shell may corrode in the presence of H_2S derived from the buffer. In a worst-case scenario, the overall corrosion rate could approximately double compared with the case in which only the outer surface is subject to corrosion.

1.2 Leakage of hydrogen through the copper overpack

This sink term is not considered in the analyses described by Bond *et al.* (1997) or Takase *et al.* (1999). It could be an important term in the CTB and CB scenarios (Takase *et al.*, 1999), however, where copper penetrations are assumed to be located above the maximum water level before hydrogen gas is vented out through the buffer. In these scenarios hydrogen gas is able to escape the system through the penetration into the bentonite buffer. With a small diameter (on the order of mm), it is possible that a gradient of hydrogen concentration forms across the copper penetration. This gradient carries hydrogen gas toward the buffer where hydrogen dissolves into the porewater and migrates away from the copper overpack via diffusion. In the following paragraphs, we estimate the mass transfer rate of hydrogen gas via gas diffusion through the penetration and aqueous diffusion within the bentonite.

First, we estimate the mass transfer rate of hydrogen gas through the copper penetration. Assuming a linear concentration gradient from one end of the penetration to the other, the mass transfer rate, F_{H2}, can be estimated using the following relation:

$$F_{\mathrm{H}_2} = A_p D \frac{C_a - C_B}{l_c}, \qquad (16)$$

where A_p stands for the cross-sectional area of the penetration (with values ranging from 5×10^{-6} to 2×10^{-5} m^2), D refers to the diffusion coefficient in the gas phase (typically 3.1557 $m^2\ yr^{-1}$), l_c = 0.05 m denotes the penetration length, and C_a and C_B represent the hydrogen concentration (mol m^{-3}) inside the annulus and at the bentonite-canister boundary, respectively.

Assuming the hydrogen concentration is related to the hydrogen pressure, $P_{H2(g)}$, inside the canister and annulus via the ideal gas law, C_a can be estimated from:

$$C_a = \frac{P_{H_2(g)}}{RT}, \quad (17)$$

where symbols are as defined above. Assuming $P_{H2(g)}$ = 5 MPa and T = 40°C, the hydrogen concentration inside the annulus and canister is equal to 1.92 mol m^{-3}. If it is also assumed that the hydrogen concentration at the bentonite-canister interface is equal to zero, the mass transfer rate of hydrogen gas out of the canister is approximately 6×10^{-4} to 2×10^{-3} mol yr^{-1}.

Second, we estimate the mass transfer rate of aqueous hydrogen through the buffer. Assuming mass transfer is controlled by diffusion, the mass transfer rate at the buffer-canister interface can be estimated using an analytical expression derived by Chambré *et al.* (1986). These investigators obtained a solution for mass transfer through a pinhole defect in a canister into a three-dimensional water-saturated porous medium. The corresponding rate, m_H, is given by:

$$m_H = 4D_f \varepsilon r_p C_c, \quad (18)$$

where D_f stands for the diffusion coefficient in liquid water (0.0315 m^2 yr^{-1}), ε denotes the buffer's porosity (40%), r_p refers to the penetration radius (0.0013 – 0.0025 m), and C_c represents the aqueous hydrogen concentration (mol m^{-3}) at the buffer-canister interface.

If we ignore gaseous diffusion of hydrogen within the penetration, we can assume the partial pressure of hydrogen at this interface is 5 MPa. According to Henry's law, the hydrogen aqueous concentration at this location is then about 40 mol m^{-3}. Substituting values into Eqn. (18) gives a mass transfer rate of approximately 0.003 to 0.005 mol yr^{-1}.

Next, we estimate the hydrogen build-up rate due to corrosion and compare this with the leakage rates estimated above. If the build-up rate is comparable with the leakage rate, then the leakage "sink term" should not be neglected in the analysis.

The following equation from Takase *et al.* (1999) is used to estimate the rate of hydrogen gas buildup, R_{H2}, within the canister and annulus:

$$R_{H2} \approx \frac{P_{H2} - P_{H2,0}}{RT\Delta t}\left(V_c + V_a\right), \quad (19)$$

where P_{H2} = 5 MPa, $P_{H2,0}$ stands for the initial hydrogen gas pressure (assumed to be equal to zero), Δt refers to the time period during which P_{H2} builds up to 5 MPa, V_c represents the interior volume of the canister (0.4 m^3), and V_a is the annulus volume (0.026 m^3). Using Δt = 8413 years for the CTB scenario with copper penetration located at the middle and top of the overpack obtained by Takase *et al.* (1999), Eqn. (19) predicts a hydrogen buildup rate of approximately 10^{-4} mol yr^{-1}.

Comparison of this result with the hydrogen-leakage rate estimated above suggests that the hydrogen sink term (controlled by aqueous diffusion out through the buffer) is greater than, or of similar magnitude to, that of the hydrogen production rate due to corrosion. This suggests that the sink term is important, and should be accounted for in analyses of the

canister-defect scenario. This term is not included in the analyses described by Bond *et al.* (1997) and Takase *et al.* (1999), however.

1.3 Water imbibition by re-consolidated bentonite

In the bentonite intrusion scenario considered by Takase *et al.* (1999), it is assumed that a continuous water pathway is maintained by capillary suction in bentonite that re-consolidates from a gel after the gel initially enters the annulus. Hence, the rate of water consumption at the corroding surface of the iron insert is controlled by the corrosion rate rather than the water-supply rate. It is questionable, however, how the re-consolidated bentonite can accommodate the water needed for the corrosion reaction. Water flow within the consolidated bentonite must obey Darcy's law even if the flow is driven by a gradient in capillary pressure. Parameters controlling this process include the hydraulic conductivity, relative permeability for liquid of the re-consolidated bentonite, and the capillary pressure gradient. If the bentonite cannot supply the water needed at the corrosion rate, there would be less hydrogen generated than estimated by Takase *et al.* (1999). If so, the importance of the "gas cushion" effect may have been over-estimated in their analysis.

2 Thermodynamic Database Supporting Calculations of Radioelement Solubilities

Solubility constraints on the source term in SR 97 are estimated by Bruno *et al.* (1997). Radioelement solubilities are calculated using the EQ3NR aqueous speciation-solubility software (Wolery, 1992) and a supporting thermodynamic database referred to as Nagra/SKB-97-TDB. The database is derived from previous databases [designated NTB 91-17 (Pearson and Berner, 1991) and NTB 91-18 (Pearson *et al.*, 1992)] combined with additional data compilations prepared by SKB for U, Pu, Tc, REE and Np. Several additions to, and modifications of, these primary data sources are described by Bruno *et al.* (1997), and are incorporated in Nagra/SKB-97-TDB. The solubilities are calculated with respect to three different groundwaters and a solution representing equilibrated bentonite porewater. The compositions of the groundwaters are based on analyses of groundwater samples from the Äspö, Finnsjön and Gideå sites.

The reliability of the Nagra/SKB-97-TDB "database" for use in performance assessments is questionable because its unclear whether the database is internally consistent. Internal consistency ensures that there are no sources of ambiguity in the database. Such ambiguities are revealed when mathematical manipulation of the data in various ways results in two (or more) different values for a given thermodynamic property. The two values are mutually incompatible, and therefore internally inconsistent with respect to the data used to calculate them. If, on the other hand, a database is internally consistent, and all such discrepancies are therefore resolved, then data that are in conflict with experimental observations can be attributed unequivocally to errors in the data, or to errors in the experimental results. Internal consistency is thus a conditional requirement, which must be met before the accuracy of a database can be unambiguously assessed.

The internal consistency of a database is best evaluated in terms of a level of increasingly stringent conditions (Engi, 1992):

- all the data are compatible with basic thermodynamic definitions, and basic functional relations used to retrieve parameter values from experimental results,

- a single set of reference values (*e.g.*, reference temperature and pressure), constants (*e.g.*, gas constant, atomic weights, *etc.*) and standard-state conventions is adhered to,

- the interdependence of the data is minimized, *e.g.*, by simultaneous evaluation of experimental data for multiple reactions, and

- parameter values are constrained by *all* relevant experimental (and field) data, except those data that are rejected (or uncertainties "relaxed") on the basis of experimental procedures employed.

Thermodynamic databases are then classified as:

- *formally* consistent if only the first two conditions are satisfied,

- *partially* consistent if the third condition is also satisfied, or

- *fully* consistent if all four conditions are satisfied.

This definition of internal consistency is useful because it includes the concept of "levels-of-attainment". A fully consistent database is thus an ideal standard, which may be extremely difficult to achieve in practice, and to maintain as the database is inevitably updated and revised. It is important to emphasize that the level of internal consistency does not necessarily correlate in any meaningful way with the accuracy of the data. Thus, thermodynamic data in an uncritical data compilation may still be accurate.

Taken at face value, the development of Nagra/SKB-97-TDB as described by Bruno *et al.* (1997) leaves considerable doubt as to whether this database is even formally consistent. The authors appear to have simply compiled preferred thermodynamic data from various sources, despite numerous cautions in the scientific literature that this is an unacceptable approach for developing a reliable thermodynamic database (Helgeson *et al.*, 1978; Berman, 1988; Holland and Powell, 1990; Grenthe *et al.*, 1992; Silva *et al*, 1995; Gottschalk, 1997; Rard *et al*., 1999). It is important to note that Bruno *et al.* (1997) do assess the accuracy of their thermodynamic data by comparing calculated solubilities with radioelement concentrations observed in natural systems and experimental solutions in contact with spent fuel. These authors have also undertaken a systematic evaluation of the effects of uncertainties in key environmental parameters (pH, redox potential, total dissolved carbonate concentrations and temperature) on calculated solubilities. Given the general importance of thermodynamics-based calculations supporting solubility calculations and numerous other aspects of SKB's SR 97 performance assessment (and future assessments of the KBS-3 disposal concept), however, SKB should undertake a more concerted effort to develop a reliable thermodynamic database for both "geoelements" and radioelements to help build confidence in the results of these calculations.

3 Near-Field Chemistry

The chemistry of the near field does not figure prominently in SR 97, except insofar as the near-field environment is considered qualitatively with regard to constraints on the long-term stability of the canister, the dissolution rate of spent fuel and the speciation-solubility-sorption behavior of radioelements released from the fuel. In contrast, near-field chemistry is significantly more important in most other international performance assessments, where the chemistry and chemical evolution of buffer porewaters is used as the basis for estimating solubility-limited constraints on the source term (McKinley and Savage, 1994). The rationale for adopting this latter approach is that the properties of bentonite-porewater systems are thought to be better characterized and more likely to be time invariant than corresponding properties of other engineered barrier components or the geosphere. SKB have apparently rejected this line of reasoning, and, if so, it would be helpful for SKB to explain why.

The chemical evolution of buffer porewaters resulting from the interaction of MX-80 bentonite with Äspö, Finnsjön or Gideå groundwaters is modeled by Bruno *et al.* (1999). The results of that study are not used in SR 97, however. Rather, a modeled porewater composition resulting from the interaction of MX-80 bentonite with a synthetic, "Allard "-type groundwater (Wanner *et al.*, 1992) is used by Bruno *et al.* (1997) to estimate near-field radioelement solubilities. If these solubilities are greater than those calculated for the Äspö, Finnsjön or Gideå groundwaters, then the near-field solubilities are conservatively used in SR 97. There is no explanation, however, why the apparently more relevant modeling results of Bruno *et al.* (1999) were not used to estimate near-field solubilities in SR 97.

The report by Bruno *et al.* (1999) does not advance the understanding of processes controlling the chemical evolution of buffer porewaters beyond that developed in previous modeling studies for SKB carried out by Wanner *et al.* (1992) and Wieland *et al.* (1994). This understanding has been criticized by Roaldset *et al.* (1996) and Savage *et al.* (1999) for several reasons, including:

- the ion-exchange/surface-complexation models of smectite-water equilibria developed by Wanner *et al.* (1992) and Wieland *et al.* (1994) are overly simplistic because they assume that reactions involving ionic substitutions on octahedral and tetrahedral sites in this mineral do not occur, despite abundant evidence to the contrary from studies of natural clay minerals in near-surface environments, and in direct contradiction of assumptions adopted by SKB in similar models of smectite illitization,

- parameters in the ion-exchange/surface-complexation models are calibrated solely on the basis of short-term experiments – the models may thus be unsuitable for predictions of long-term behavior (Arthur and Wang, 1999), and

- the "mixing-tank" model used by Wanner *et al.* (1992) and Bruno *et al.* (1999) to simulate continuous interaction of the buffer and site groundwaters over long periods of time is overly simplistic because it fails to account for diffusional rather than advective solute transport into, or out of, the buffer.

The fact that modeling approaches other than those adopted by Wanner *et al.* (1992) and Wieland *et al.* (1994) have been developed for clay minerals is acknowledged by Bruno *et al.* (1999). Some of these alternative approaches are also described in the "Process Report" (SKB, 1999b). There has been no effort by SKB, however, to evaluate whether these alternative approaches could be used to advantage in models of bentonite-water interaction. Reasons for this remain unclear.

4 Ice Melting and Redox-Front Migration

The potential for oxygenated solutions resulting from the melting of an ice sheet to migrate to repository depths is mentioned in several places in the summary and main reports documenting SR 97 (SKB, 1999a). A modeling study commissioned by SKB (Guimerà *et al.,* 1999) and independently reviewed by Gascoyne (1999) basically confirms earlier analyses by Arthur (1996) and Glynn and Voss (1999) indicating that this scenario is possible, although unlikely.

Guimerà *et al.* (1999) seem to imply that the stationary-state modeling approach used by Arthur (1996) is limited to consideration of equilibrium processes. Arthur (1996) emphasizes, however, that the approach accounts explicitly for both reaction kinetics and the groundwater flow rate. Guimerà *et al.* (1999) also do not acknowledge the work of Glynn and Voss (1999), which includes a summary of direct field evidence implicating the migration of oxygenated solutions to depths exceeding those considered in the KBS-3 concept. The importance of this process with regard to repository performance is discussed in Section 10.10.3 of SKB (1999a), where it is again concluded that the likelihood of oxygenated solutions migrating to repository depths is remote. It is important to bear in mind that the conclusions of all the studies noted above are based on scoping calculations using simplified models of complex hydrochemical-hydrogeologic processes driven by a climate-change scenario. For this reason, the recommendation of Arthur (1996) and Glynn and Voss (1999) to examine rock and groundwater samples currently in hand, or that will be obtained in the future, for evidence of past migration of oxygenated solutions in the deep subsurface is still appropriate.

5 References

Adamson, A. W. 1967. *Physical chemistry of surfaces, 2nd ed.* Interscience, Publ., New York, 747p.

Arthur, R. C. 1996. Estimated rates of redox-front migration in granitic rocks. SKI Report 96:35, Swedish Nuclear Power Inspectorate, Stockholm, Sweden.

Arthur, R. C. and Murphy, W. M. 1989. An analysis of gas-water-rock interactions during boiling in partially saturated tuff. *Sci. Géol. Bull.,* 42 (4), 313-327.

Arthur, R. C. and Wang, J. 1999. Claystone constraints on models of the long-term chemical evolution of buffer porewaters. In. *Scientific Basis for Nuclear Waste Management XXIII* (R.W. Smith and D. Shoesmith, eds.), Mat. Res. Soc. Symp. Proc. (in press).

Berman, R.G. 1988. Internally-consistent thermodynamic data for minerals in the system Na_2O-K_2O-CaO-MgO-FeO-Fe_2O_3-Al_2O_3-SiO_2-TiO_2-H_2O-CO_2. *Journal of Petrology*, 29(2),445-522.

Blackwood, D. J., Hoch, A. R., Naish, C. C., Rance, A. and Sharland, S. M. 1994. Research on corrosion aspects of the advanced cold process canister. SKB TR 94-12. Swedish Nuclear Fuel and Waste Management Co., Stockholm, Sweden.

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

Bruno, J., Cera, E., de Pablo, J., Duro, L., Jordana, S. and Savage, D. 1997. Determination of radionuclide solubility limits to be used in SR 97: Uncertainties associated to calculated solubilities. SKB TR 97-33. Swedish Nuclear Fuel and Waste Management Co., Stockholm, Sweden.

Bruno, J., Arcos, D. and Duro, L. Processes and features affecting the near field hydrochemistry: Groundwater-bentonite interaction. SKB TR 99-29, Swedish Nuclear Fuel and Waste Management Co., Stockholm, Sweden.

Chambré, P. L., Lee, W. W-L., Kim, C. L. and Pigford, T. H. 1986. Steady-state and transient radionuclide transport through penetrations in nuclear waste containers. LBL-21806/UC-70, Lawrence Berkeley Laboratory, Berkeley, CA.

Drummond, S. E. 1981. Boiling and mixing of hydrothermal fluids: Chemical effects on mineral precipitation. Unpubl. Ph.D. Diss., Pennsylvania State Univ., 357p.

Drummond, S. E. and Ohmoto, H. 1985. Chemical evolution and mineral deposition in boiling hydrothermal systems. *Econ. Geol.*, 80, 126-147.

Engi, M. 1992. Thermodynamic data for minerals: a critical assessment. In: *The stability of minerals* (G.D. Price and N.L. Ross, eds.), Chapman & Hall, London, 267-328.

Gascoyne, M. 1999. Long-term maintenance of reducing conditions in a spent nuclear fuel repository: A re-examination of critical factors. SKB R-99-41. Swedish Nuclear Fuel and Waste Management Co., Stockholm, Sweden.

Glynn, P. D. and Voss, C. I. 1999. Geochemical characterization of Simpevarp ground waters near the Äspö hard rock laboratory. SKI Report 96:29, Swedish Nuclear Power Inspectorate, Stockholm, Sweden.

Gottschalk, M. 1997. Internally consistent thermodynamic data for rock-forming minerals in the system SiO_2-TiO_2-Al_2O_3-Fe_2O_3-CaO-MgO-FeO-K_2O-Na_2O-H_2O-CO_2. *Eur. J. Mineral.*, 9, 175-223.

Grenthe, I., Fuger, J., Konings, R.J.M., Lemire, R. J., Muller, A. B., Nguyen-Trung, C. and Wanner, H. 1992. *Chemical thermodynamics of uranium*. Elsevier Science Publ., Amsterdam, 715p.

Guimera, J., Duro, L., Jordana, S. and Bruno, J. 1999. Effects of ice melting and redox front migration in fractured rocks of low permeability. SKB TR 99-19. Swedish Nuclear Fuel and Waste Management Co., Stockholm, Sweden.

Helgeson, H.C., Delany, J.M., Nesbitt, H. W., and Bird, D.K. 1978. Summary and critique of the thermodynamic properties of rock-forming minerals. *Am. J. Sci.*, 278-A, 1-229.

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

Holland, T.J.B. and Powell, R. 1990. An enlarged and updated internally consistent thermodynamic dataset with uncertainties and correlations: the system K_2O-Na_2O-CaO-MgO-MnO-FeO-Fe_2O_3-Al_2O_3-TiO_2-SiO_2-C-H_2BO_2. *J. Metamorphic. Geol.*, 8, 89-124.

Johnson, A. B. Jr., and Francis, B. 1980. Durability of metals from archaeological objects, metal meteorites, and native metals. PNL-3198 UC-70, Battelle, Pacific Northwest Laboratories, Richland, Washington.

McKinley, I. and Savage, D. 1994. Comparison of solubility databases used for HLW performance assessment. *Fourth intl. conf. on the chemistry and migration behavior of actinides and fission products in the geosphere*. R. Oldenburg Verlag Publ., München, 656-665.

Miller, W., Alexander, R., Chapman, N., McKinley, I. and Smellie, J. 1994. *Natural analog studies in the geological disposal of radioactive wastes*. Studies in Environmental Sciences, 57, Elsevier, New York.

Neretnieks, I. 1985. Some aspects of the use of iron canisters in deep lying repositories for nuclear waste. Nagra TR 85-35. Nagra, Baden, Switzerland.

Pearson, F. J., Jr. and Berner, U. 1991. Nagra thermochemical data base I. Core data. Nagra TR 91-17, Nagra, Baden, Switzerland.

Pearson, F. J., Jr., Berner, U. and Hummel, W. 1992. Nagra thermochemical data base II. Supplemental data. Nagra TR 91-18, Nagra, Baden, Switzerland.

Platts, N., Blackwood, D. J. and Naish, C. C. 1994. Anaerobic oxidation of carbon steel in granitic groundwaters: A review of the relevant literature. SKB TR 94-01. Swedish Nuclear Fuel and Waste Management Co., Stockholm, Sweden.

Rard, J. A., Rand, M. H., Anderegg, G. and Wanner, H. 1999. *Chemical thermodynamics of technetium*. Elsevier Science Publ., Amsterdam, 568p.

Roaldset, E., Sällfors, G. and Arthur, R. 1996. Förstudie beträffande bentonitens roll i ett slutförvar för radioaktivt avfall. SKI Report 96:44, Swedish Nuclear Power Inspectorate, Stockholm, Sweden.

Savage, D., Lind, A. and Arthur, R. C. 1999. Review of the properties and uses of bentonite as a buffer and backfill material. SKI Report 99:09, Swedish Nuclear Power Inspectorate, Stockholm, Sweden.

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

Silva, R. J., Bidoglio, G., Rand, M., Robouch, P. B., Wanner, H. and Puigdomenech, I. 1995. *Chemical thermodynamics of americium*. Elsevier Science Publ., Amsterdam, 374p.

SKB 1999a. Deep repository for spent nuclear fuel: SR 97 – Post-closure safety: Main report summary, main report volumes I and II. SKB TR 99-06. Swedish Nuclear Fuel and Waste Management Co., Stockholm, Sweden.

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

Wanner, H., Wersin, P. and Sierro, N. 1992. Thermodynamic modeling of bentonite-groundwater interaction and implications for near field chemistry. SKB TR 92-37, Swedish Nuclear Fuel and Waste Management Co., Stockholm, Sweden.

Wieland, E., Wanner, H., Albinsson, Y., Wersin, P. and Karnland, O. 1994. A surface chemical model of the bentonite-water interface and its implications for modeling the near field chemistry in a repository for spent fuel. SKB TR 94-26, Swedish Nuclear Fuel and Waste Management Co., Stockholm, Sweden.

Wolery, T. J. 1992. EQ3NR, A computer program for geochemical aqueous speciation-solubility calculations: Theoretical manual, user's guide, and related documentation (Version 7). UCRL-MA-110662 PT III, Lawrence Livermore National Laboratory, Livermore, CA.

The authors

Randy Arthur

Dr. Arthur obtained his Ph.D. from the Pennsylvania State University in the field of geochemistry and mineralogy. He has over nineteen years' experience in geochemical investigations supporting site selection, site characterization and performance assessments of geologic repositories for radioactive and hazardous wastes. Dr. Arthur has been lead investigator on a number of laboratory, field and geochemical modeling projects for commercial and national R&D organizations in Japan, Sweden, France, Switzerland and the U.S. The scope of the projects ranges from characterization of the chemistry of deep groundwaters in highly fractured crystalline rocks to testing and analyses of materials for use as engineered barriers to radionuclide migration from deep geologic repositories for nuclear wastes. Dr. Arthur's expertise also extends to the critical evaluation and retrieval of thermodynamic and kinetic data from experimental investigations, and compilation of these data into internally consistent databases. Dr. Arthur has served as a technical expert in the area of geochemistry in support of safety assessments of geologic disposal concepts for nuclear wastes in Japan, Sweden and the U.S. He has presented and/or published over 50 papers in peer-reviewed journals and symposia proceedings, as well as numerous technical reports published by national R&D organizations in the U.S., Europe and Asia.

Wei Zhou

Dr. Wei Zhou received her Ph.D. from the University of California, Berkeley in the field of nuclear engineering. She has ten years' post-graduate experience in risk, safety, and environmental impact assessments supporting hazardous and nuclear waste management. Dr. Zhou has participated in several multinational R&D programs addressing deep geologic disposal concepts for nuclear wastes. Her support to these programs includes development of a Total System Performance Assessment methodology and associated software for the near-field at Yucca Mountain, Nevada, coupled process modeling, simulation of gas migration in the geosphere, modeling of flow and transport in fractured rock, scenario analysis, uncertainty analysis, EBS analysis and design, and long-term safety assessments of deep geologic repositories for nuclear wastes. Dr. Zhou has authored or co-authored over 40 peer-reviewed papers and technical reports.

Evaluation of SR 97 Regarding Treatment of Uncertainties in Chemical Systems

Christian Ekberg

Department of Nuclear Chemistry
Chalmers University of Technology
S-412 96 Göteborg, Sweden

Aim

The aim of this review is to evaluate the SKB safety report SR 97 with respect to the handling of uncertainties related to chemical modelling together with a glance at the handling of the general chemistry.

Introduction

Today, one can often find work reported in the scientific literature in which computer simulations are made instead of experiments, especially in areas where experiments are difficult, expensive or impossible to conduct. One of the latter is to try to foresee what happens in the future with a repository for spent nuclear fuel which have to be functioning for very many years. It is not uncommon that the data used in calculations and simulations related to this very difficult topic are questionable for some reason. The result of this is that the outcome of the calculations will always be more or less uncertain. This fact enhanses the importance of uncertainty and sensitivity analysis, which has attracted greater and greater attention in the scientific community during the last years. Several conferences in the subject have become more open for the common researcher, e.g. PSAM (Probabilistic Safety Assessment and Management) and SAMO (Sensitivity Analysis of Model Output). Unfortunately, there still seems to be some resistance to abandon the traditional methods, which only gives one deterministic answer, which may be right or wrong depending on how it is used. Basing important decisions on a fixed result, which does not give any clue about the inherent uncertainty, is in my opinion unsatisfactory as evidence that a repository for spent nuclear fuel is safe. The uncertainties entering into every calculation (and experiment) should be given some kind of scientific treatment. Depending on the origin of the uncertainty several methods to achieve this are described in the literature, e.g. [HEL 97], KLE[95] and [EKB 95].

For the case of chemical modelling (and in other cases) it is possible to distinguish some different types of uncertainties. The first of these (and in many cases the greatest) is the conceptual uncertainty. It reveals the fact that there may be several methods to quantify a specific phenomenon or a combination of phenomena, and these different methods produce different results. At a first glance, it may seem trivial to distinguish which models or results are “right” or which are “wrong” for a particular context but unfortunately in many cases this is not the reality. Other important types of uncertainties are those that affect the derivation of input data used for the modelling. These may usually be treated with some of the methods existing in the literature, such as statistical methods or response surface methods.

Comments

Reading SR 97 revealed that some comments need to be made regarding the treatment of uncertainties. Additional comments related to the handling of the general chemistry are also provided, e.g. chemical speciation which deserve some enlightening (see below).

The fact that it is impossible to show that all variables, processes and connections in a safety assessment have been taken into account is elementary and does not need be further addressed. However, it must be up to SKB to prove that their decisions and judgements are within reason. For example, it is written in chapter 4.6.3 in the main report that overestimating the ”risks” may compensate lack of detailed knowledge. One can argue that is a questionable approach. For instance, there may be situations, e.g. in non-linear solubility calculations, where several input data with values assumed to be conservative may give a relatively low solubility. However, a combination

of parameter values where some are assumed to be conservative and some realistic may give a higher solubility. This is an effect of correlations and an analysis of these is very important. Such an analysis requires a detailed knowledge of the individual processes and the equations used to simulate these.

Conceptual uncertainties

Conceptual uncertainties are discussed in a satisfactory, but somewhat too brief, way in chapter 4.6.3 in the main report. Unfortunately, there is no description about what SKB are planning to do about these uncertainties. It is not enough only to discuss the reliability of the models (validation). One should also discuss the comparison between the different conceptual models that are available for the specific problem. In addition, one should also try to invalidate the models, i.e. showing where they are definitely wrong. All models have a validity range and it is important to identify and describe this range [NOR 92]. The simplest method is probably to solve the problem with different models, then discuss the differences and finally draw the conclusions based on those discussions.

Statistical uncertainty analysis

The discussions made regarding conditioned and unconditioned probabilities in chapter 4.6.5 are reasonable. My only problem is how to put a figure on "consequence". This has not been described in SR 97 and thus I assume that they are based on subjective judgements. The use of probabilistic methods in SR 97 is exemplified by determination of the solubilities for the different radionuclides, see chapter 4.6.5 in the main report. There it is stated that "It has been extremely difficult to give a reliable distribution of possible values for the solubilities". Although this is completely true, the preferred method in such a case should be to use an uniform distribution for a wide interval and thus increase the probability that "points" in the tails of the distributions are included, see the discussion below.

Until today only one SKB-report has been published [BRU 97] that explicitly mention the handling of uncertainties in solubility calculations. This report also includes the derivation of solubilities used in SR 97. In this report, the treatment of the general chemistry is, according to my judgement, of good quality . However, keeping in mind what has been done in the rest of the world in the context of uncertainty and sensitivity analysis, e.g. England and USA [HAW 98][HEL 97][EKB 98], the handling of the uncertainties in this report is at the best rudimentary. The approach of using only one "low" and one "high" value for a given variable when judging its importance is not enough. Chemical speciation is in most cases not linear why the adopted procedure in SR 97 only gives a rough estimate, at the best. A more preferable method is to work from the bottom and upwards in the investigation. This means that an uncertainty analysis of e.g. radionuclide transport starts with the effects and role of different uncertainties in the solubility calculations. The results from these probabilistic solubility calculations will then be the probabilistic input for the further transport calculations.

As an example of the handling and recognition of uncertainties it may be worth mentioning a part of chapter 4.6.3, which is dealing with the illitisation of the buffer material. According to SKB the extent of this process may be estimated if the availability of potassium is known. This is probably true but then it is also claimed that the amount potassium may be easily calculated. This is in my opinion not at all evident. It is not shown which uncertainties that need to be considered in such a calculation,

keeping in mind the amount of potassium in the repository and in the future ground water composition, which is also needed as a basis for the solubility calculations.

The discussion made in connection with distributions is bantering and rather irrelevant (although correct). It is said that since it is not possible to get distributions for all parameters and thus they are excluded from the probabilistic calculations by assuming that they can be represented by only two values. A more "conservative" method would have been to assume uniform distributions for the radionuclide solubilities concerned and thus enhance the probability that solubilities far from the mean value would occur. The slightly inadequate method used in SR 97 make the conclusions regarding solubilities slightly suspicious. If there are no reliable probability distributions available it is even more essential that their importance is evaluated. As mentioned above, one can always assume a uniform distribution and assign to it a range of about two times what is perceived as a realistic interval based on the limited information that is available.

According to SKB, probabilities are supposed to be allocated to the data so the "risk " is overestimated. I can not see how this can be demonstrated in a satisfactory way. However, even if the method of risk analysis adopted in SR 97 is questionable, many positive features of SR 97 balance this shortcoming. An example that it is worth mentioning is the results from the unrealistic but extremely conservative calculation cases with e.g. immediate dissolution of the fuel and no diffusion resistance within the buffer material, which are presented in chapter 9.11.10. It is useful to demonstrate that consequences are rather limited even when a "worst case" is discussed.

Chemical speciation

Chemical speciation and the uncertainties associated herewith are almost neglected or are at least not considered in sufficient detail. In chapter 9.11 in the main report I did not even find the word speciation although it is crucial for phenomena such as sorption and solubility limitations. The solubility of an element is directly dependent on the speciation since the more of a complex that can to formed, the more of the element concerned will be in solution and thus a higher solubility should be used in the performance assessment. The same is true for sorption and surface complexation. One must also consider that the same element can sorb differently on the same surface due to the differences in the chemical environment that are assumed to exist in the rock. The resulting solubilities and sorption coefficients are then used in the modelling of the radionuclide transport. Since SKB has used only a very limited number of reference waters that are supposed to be valid for many possible cases and scenarios, this method can be regarded as inflexible. An alternative approach is to predict the chemical composition of a groundwater based on the composition of a rock sample, groundwater flow etc. and then use these results to calculate the solubilities and the sorption coefficients of interest. Such a method would, make a more thorough uncertainty and sensitivity analysis possible. The latter would indicate which factors are of importance and need to be studied further. Naturally, also this method has some drawbacks, e.g. it is necessary to include a larger number of uncertain parameters in the system. These, on the other hand, may be handled by probabilistic modelling [HEL 93][HEL 94].

Finally it is worth mentioning that a too large part of the references given in SR 97 are to internal SKB reports. This could have a negative impact on SKB's credibility, although these reports generally keep a very good standard. By referring to internal reports, SKB gives the opponents the possibility to claim that SKB are biased and do not pay sufficient attention to international experts. It

would have been better to refer to the open scientific literature to a larger extent in order to increase the general credibility.

References

BRU 97 Bruno, J., Cera, E., de Pablo, J., Duro, L., Jordana, S., Savage, D., ”Determination of radionuclide solubility limits to be used in SR 97. Uncertainties associated to calculated solubilities”, SKB TR 97-33, Svensk Kärnbränslehantering AB, 1997.

EKB 95 Ekberg, C., ”Uncertainties in Safety Analysis, A Literature Review”, SKI Report 95:17, ISSN 1104-1374, ISRN SKI-R--95/17--SE, Swedish Nuclear Power Inspectorate, 1995.

EKB 98 Ekberg, C., Emrén, A. T., "Uncertainties in solubility calculations aimed at a repository for spent nuclear fuel.", Proceedings of the PSAM 4 conference, 13-18 September, New York City,vol. 4, p.2223-2228, 1998

HAW 98 Haworth, A., Thompson, A. M., Tweed, C. J., “ Use of the HARPROB Program to Evaluate the Effect of Parameter Uncertainty on Chemical Modelling Predictions”, Radiochim. Acta, 82, pp. 429-433, 1998.

HEL 93 Helton, J. C., " Uncertainty and sensitivity analysis techniques for use in performance assessment for radioactive waste disposal", Rel. Eng. and System Safety, vol. 42, pp. 327-367, 1993.

HEL 94 Helton, J. C., "Treatment of Uncertainty in Performance Assessments for Complex Systems", Risk Analysis, Vol. 14, no. 4, 1994.

HEL 97 Helton, J. C., "Uncertainty and Sensitivity Analysis in the Precence of Stochastic and Subjective Uncertainty", Journal of Statistical Computation and Simulation, vol. 57 (1-4), p. 3-76, 1997.

KLE 95 Kleijnen, J. P. C., “Sensitivity Analysis, Uncertainty Analysis, and Validation: a Survey of Statistical Techniques and Case Studies.”, Proceedings of the Symposium on Theory and Applications of Sensitivity Analysis of Model Output in Computer Simulations (SAMO), Belgirate, Italy, September, 1995.

NOR 92 Nordstrom, D. K., "On the Evaluation and Application of Geochemical Models.", Proceedings of the fifth CEC Natural Analogue Working Group Meeting EUR 15176, Toledo, 5-9 Oct., 1992.

The author

Christian Ekberg
Christian obtained his PhD in nuclear chemistry in March 1999 with the thesis "Uncertainties in Actinide solubility Calculations Illustrated using the Th-OH-PO_4 System". During the scope of this thesis mainly two areas were covered: statistics and basic chemistry combined with thermodynamics. The statistical part included the development and then use of computer programs for handling of uncertainties in chemical modelling. The experimental part was focused around determination of various stability constants for thorium. The methods used included both potentiometric titrations and solvent extraction.

During his time at the Department of Nuclear Chemistry, Christian has been active in several projects not directly related to his own PhD work. Among these are: separation and transmutation of spent nuclear fuel, the effects of cement on the chemical environment in an underground repository, computer simulation of parameters for the production of super heavy elements, the effect of different factors on the growth of algae, methods for determination of yeast metabolism, coupled reactive transport models for rock water interactions and calculations for severe reactor accidents such as core melt downs.

After the dissertation Christian has made a post-doc at the Australian Nuclear Science and Technology Organisation (ANSTO). There he studied the hydrolysis of uranium(IV) and zirconium. During this time he also suggested a new method for simultaneous detection of organic and aqueous phases using an ICP-MS.

Now, Christian is mainly working with further development of his computerised uncertainty and sensitivity analysis tools, determination of hydrolysis constants for Zr, U(IV) and Np(IV) together with co-supervising four PhD students.

Review Comments
on the
SR 97 Post-Closure Safety Assessment

Joel Geier
Oregon State University
Corvallis, OR 97331, USA

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Summary

These review comments concern an assessment of the long-term safety of a deep repository for spent nuclear fuel, titled Safety Report 97 (SR 97), which was prepared by the Swedish Nuclear Fuel Waste Management Company (SKB). The primary focus of this review is on hydrogeologic issues relating to groundwater flow, hydrologic uncertainty, and the potential for radionuclide transport from leaking canisters.

The main hydrological model that was used in SR 97 is based on a continuum conceptual model of groundwater flow in fractured bedrock. Major problems with this model include the following:

- The validity of the continuum model is arguable for the type of rock that is present at these sites.

- The suitability of the model for the intended purpose of predicting streamlines and travel times for groundwater flow through the rock mass has not been adequately demonstrated.

- The comparison with alternative, discrete models yielded more divergent results than has been recognized in the SR 97 reports.

- The comparison with alternative models did not consider significant, realistic sources of uncertainty in the alternative models, evaluation of which would have likely led to greater divergence.

The SR 97 model of radionuclide transport is based on a 1-D streamtube formulation, within which the predicted release of radionuclides to the biosphere is dominated by a parameter called the *F* ratio. A key factor in this parameter is the flow wetted surface. All of the hydrologic models used in SR 97 relied upon essentially the same set of geometric assumptions to estimate flow wetted surface from conductive fracture frequency in boreholes. Hence the predictions of the alternative models are not independent. Alternative methods of estimating flow wetted surface are needed to obtain a realistic evaluation of the uncertainty regarding radionuclide release.

The alternative 3-D hydrologic models were used only to predict streamtube parameters, not for actual transport simulations. Hence the comparison between the main hydrologic conceptual model and alternative models does not include a full assessment of the effects of flow field complexity on radionuclide transport. As this is one of the major distinctions between the continuum model and the alternative models, the comparison must be regarded as incomplete.

Besides these major hydrological issues, miscellaneous comments are offered on aspects of the repository system design and site descriptions that relate to hydrology.

Contents

1. Introduction

The Swedish Nuclear Fuel Waste Management Company (SKB) recently presented an assessment of the long-term safety of a deep repository for spent nuclear fuel, titled Safety Report 97 (SR 97). The analysis considers three alternative, hypothetical sites referred to as Aberg, Beberg, and Ceberg, which for the purposes of SR 97 are considered to be generic (fictional) sites but represented by site-specific data from the Äspö, Finnsjön, and Gideå study sites in Sweden.

This report presents comments based on a review of selected aspects of SR 97. The review was requested by the Swedish Nuclear Power Inspectorate (SKI). A summary of the author's technical background related to radioactive-waste disposal issues is given in Appendix 1.

2. Scope

This review was based primarily on the SR 97 main report series consisting of the SR 97 Main Report (Volumes I and II) and the three main supporting reports referred to by SKB as the “Design Report”, the “Processes Report” and the “Data Report”.

The primary focus of this review was hydrogeologic and transport issues, specifically with regard to groundwater flow, hydrologic uncertainty, and the potential for radionuclide transport from leaking canisters. Background reports describing the site-scale hydrogeologic models and “alternative” hydrologic models were reviewed to assess questions that followed from the review of the main report series. Other aspects of the safety assessment such as repository design, formulation of scenarios, and seismic hazard assessment, as presented in the main report series, were also reviewed with attention to hydrologic issues and implications.

3. Groundwater flow model

The primary model for groundwater flow in SR 97 is a stochastic continuum model, implemented in the HYDRASTAR code. Four major problems can be identified regarding this model:

- *The validity of the continuum model is arguable for the type of rock that is present at these sites.*

- The suitability of the model for the intended purpose of *predicting streamlines and travel times for groundwater flow through the rock mass* has not been adequately demonstrated.

- The comparison with alternative models yielded more divergent results than has been recognized in the SR 97 reports.

- The comparison with alternative models did not consider significant, realistic sources of uncertainty in the alternative models, evaluation of which would have likely led to greater divergence.

These problems are discussed in detail in the following subsections.

3.1 Validity of the continuum model

Major comments

Continuum models (PHOENIX and HYDRASTAR) have been used as the primary method for hydrogeological analysis in SR 97. The scientific basis for this type of model, for sparsely fractured crystalline rock such as within the repository blocks of the sites considered here, is much weaker than has been acknowledged in the SR 97 report series.

Questions as to the applicability of the continuum approach for sparsely fractured rock similar to the rock at these sites have motivated a large body of research (National Research Council, 1996). For two of these sites specifically (Aberg and Beberg), past discrete-fracture network modeling has indicated that the continuum assumption may not be appropriate on the scale of emplacement holes or the blocks in the HYDRASTAR model. The limited calibration studies and comparisons with alternative hydrogeologic models are not sufficient to establish that the continuum models are valid for the purposes that they have been used for in SR 97.

Questions about the validity of the continuum approach are significant for the safety assessment, because the continuum models are used to extrapolate long-term hydrologic conditions on varying scales from a spatially and temporally restricted set of hydrologic measurements. The models are used to predict groundwater flux through emplacement holes, and groundwater paths and travel times from leaking canisters to the biosphere. These predictions are used, in turn, to predict the effectiveness of the geosphere for radionuclide retention. If the underlying conceptual model for groundwater flow is not valid for the type of rock that exists at these sites, this may lead to gross errors in the predictions of radionuclide retention, especially for future groundwater conditions that differ from the narrow range of conditions for which the models were calibrated.

Elaboration of major comments

Contrary to the statement that appears in the discussion of conceptual uncertainties for HYDRASTAR [SR 97 Main Report, Vol. II, p. 297], the description of groundwater flow in terms of a 3-D form of Darcy's law is not well founded for the case under consideration, *i.e.* groundwater flow through *sparsely fractured crystalline rock*. Questions as to the applicability of Darcy's law for this type of rock have motivated a large body of research on other modeling approaches (National Research Council, 1996). These questions need to be acknowledged and dealt with in the safety assessment.

The fundamental groundwater-flow phenomenon in fractured, crystalline rock is viscous flow through discrete fractures of variable aperture (in the worst case, discrete channels). Flow in a single, open fracture can be described in terms of the Navier-Stokes equations. Flow through a network of intersecting fractures is further constrained by conservation of mass and continuity of pressure at fracture/channel intersections.

Much experimental and theoretical research (see, e.g., National Research Council, 1996) has been devoted to determining the conditions under which the process of flow through a single fracture can be described in simpler terms (as opposed to the full Navier-Stokes equations), e.g. by a 2-D form of Darcy's law that applies only within the plane of the individual fracture. Most discrete-network models, including the discrete-fracture network (DFN) and channel-network (CN) models that were used in the "alternative models project," make use of this type of simplification.

The main site-scale groundwater flow model that was employed in SR 97, HYDRASTAR, is a continuum model. Adoption of a continuum model involves a further simplifying assumption which is not stated explicitly in the SR 97 main report series: *It is assumed that groundwater flow through fractured crystalline rock at these sites can be described in terms of Darcy's law for flow through an equivalent porous medium.*

In essence this means that, for the blocks in the HYDRASTAR model, it is assumed that each block can be described in terms of an equivalent block of porous medium that has a material property (permeability, whether a scalar or a tensor value) that is independent of the direction of flow and the hydraulic boundary conditions.

Darcy's law is well established as an empirical law that describes flow through well-connected porous media such as sediments and sedimentary rock, where the continuum assumption is generally considered to be valid. However, there is little or no empirical evidence that the continuum assumption is valid for sparsely fractured crystalline rock. Experiments to test this "law" directly would be difficult, as one would need to somehow hydraulically isolate (or alternatively, fully instrument the boundaries of) multiple rock "samples" on a sufficiently large scale such that the "samples" are representative of the range of scales over which discrete fractures/channels intersect to form a connected "pore space."

In the absence of direct empirical evidence to support the continuum assumption, attempts have been made to rationalize the use of continuum models by modeling flow through networks of discrete fractures. Generic modeling studies by Long et al. (1982) indicate that in fractured rock it may not be possible to define an equivalent permeability tensor, let alone an equivalent permeability value (scalar) such as is assumed in the isotropic form of Darcy's law, as set forth on p. 179 of the Processes Report.

Past applications of discrete-fracture network models to the Aberg site (Axelsson et al., 1989) have indicated that, on scales of 25 m and 50 m, many rock blocks show behaviors that could not be represented by an equivalent isotropic continuum. For example, some simulated blocks permitted groundwater flow in one direction but not in a perpendicular direction, and in general the calculated values of permeability, when obtained, were highly sensitive to the imposed boundary conditions.

Discrete-fracture network modelling of the Beberg site by this reviewer (Geier et al., 1992, p.169) suggested that the rock mass does not behave as an equivalent porous

medium on the 40 m block scale, although the continuum assumption was not explicitly tested. The sections of the SR 97 reports that relate to this issue do not mention any more recent studies that would give stronger support to the application of the continuum conceptual model.

The statement that "permeability … cannot normally be obtained for a fractured medium" [Processes Report, p. 182] appears to be an acknowledgement of the difficulty in demonstrating that the fractured rock at these sites behaves as a equivalent continuum. However, the assertion that "it is necessary to assign flow properties to individual fractures or rock blocks" sidesteps the crucial question of whether assignment of (effective) flow properties to the rock blocks in a continuum model will yield a valid description of the flow system, or even one that is suitable for the intended purpose of predicting streamtube properties for radionuclide transport.

A more direct and accurate discussion of the process of groundwater flow, for fractured crystalline rock, was given as an example FEP description in the earlier SKB report by Skagius et al. (1995, pp. C-4 and C-5). This description discusses several key differences between a stochastic continuum model and poorly percolating networks or the case of extreme channeling, and mentions several implications of these differences for radionuclide transport. This type of treatment would be much more direct and informative than the description of groundwater flow that appears in the Processes Report.

Detailed comments

The section **Calculation of groundwater flow** [SR 97 Processes Report, p. 179] describes a particular modeling approach (continuum approximation based on an assumption that Darcy's law applies), not the physical process of groundwater flow through fractured crystalline bedrock. This way of presenting the topic tends to obscure some of the most important issues in the evaluation of groundwater flow, as it concerns radionuclide transport.

The statement that Darcy's law is "[t]he most common approach for calculating groundwater flows in the geosphere" [SR 97 Processes Report, p. 179] is misleading, as it promotes a false impression that the conceptual model that has been adopted as the basis for the primary hydrogeological model is firmly established for this type of rock.

To say that "the choice of [hydrogeologic] model depends on the purpose of the analysis, … [the] scale …, and available data" [Processes Report, p. 185], ignores a fundamental question as to whether the chosen (continuum) model has been demonstrated to be valid for the rock type that is under consideration, on either empirical or theoretical grounds. Choice of a groundwater model must not be based simply on practical considerations such as "purpose, scale, and available data." If there is a question as to the validity of a particular model for describing the physical processes that prevail at the scale of the model, then there needs to be a demonstration of the model's validity for the intended

purposes. The Alternative Models Project appears to be an effort in that direction, but is not sufficient given the significance of this issue.

3.2 Suitability of the model for predicting streamlines and travel times

Major comments

The suitability of the continuum model for the intended purpose of predicting streamlines and travel times for groundwater flow through the rock mass has not been adequately demonstrated. This is significant, in view of the fact that the conceptual basis for the application of continuum models to sparsely fractured crystalline rock is arguable.

Contrary to statements in the SR 97 Main Report, an inverse-modeling exercise that was conducted did not provide a meaningful test of the model's conceptualization for the rock mass. The exercise did not test the model against data that were not directly used in the calibration. The exercise did not directly test the model's suitability for the type of predictions that it was used for in the safety assessment. Furthermore, the calibration dataset that was used for both calibrations and comparisons in this exercise was arguably not sensitive to rock mass hydrologic properties; rather it reflects mainly the properties of the fracture zones.

Elaboration of major comments

The SR 97 Main Report [Vol II, p. 293] states that modeling of field tests at Aberg by Walker et al. (1996) "indicates that HYDRASTAR can explain observed conditions on the site." The report goes on to state that "[t]his also suggests that HYDRASTAR'S conceptualization is suitable for its purpose."

The cited work (Walker et al., 1996) was an inverse-modeling exercise, which demonstrates only that the model is able to reproduce a subset of the cross-borehole head responses that were observed in a single, large-scale pumping test, LPT2. Agreement was achieved in the sense that the ensemble of results bounds most of, but not all of the actual observations of transient head response. No comparisons are presented with other variables that are of more direct interest for assessing the model's ability to predict transport pathways and travel times through the geosphere (for instance, the results of tracer tests in LPT2).

Results from some boreholes were excluded from the comparison for various reasons, including perceived limitations in the model's ability to represent the physical boundary conditions around the pumped borehole, near the edges of the model, near the surface where unconfined effects may prevail, and in certain borehole sections where anomalously strong connections to surface waters are thought to exist (Walker et al., 1996, pp. 26 & 43).

Anomalously strong connections in the bedrock are a matter of paramount concern for radionuclide transport. If a model cannot be made to simulate these where they are known to exist, this diminishes our confidence in the capability of the model to represent them elsewhere.

The calibrated model was assessed by comparison to the same dataset that was used directly in the pilot-point calibration. Hence this cannot be regarded as a validation exercise. This type of exercise only shows that the model possesses sufficient degrees of freedom to match most characteristics of the dataset. It does not demonstrate that the model is useful for predicting the flow fields resulting from hydrologic conditions that differ substantially from the conditions that were induced during the calibration case (the LPT2 test).

A more rigorous validation exercise than this would be needed to support the contention that "HYDRASTAR's [continuum] conceptualization is suitable for its purpose." In particular, since the major purpose of HYDRASTAR is to predict streamlines (particle trajectories) and water travel times for use in transport models, it should be demonstrated by comparison with field data that the continuum model yields satisfactory predictions of transport paths for situations that are analogous to the release of radionuclides from canisters in sparsely fractured rock. Obtaining suitable field data for validating the SC approach should be considered prior to using this approach for an actual performance assessement.

Finally, the calibration case is based on a pumping and tracer test that was designed primarily to test the hydrologic and transport properties of selected major fracture zones at the site. The limitations of the LPT2 dataset for testing hydrologic models of the more sparsely fractured rock, such as the deposition blocks, have previously been discussed by this reviewer (Geier, 1996). An ability to reproduce the main features of the LPT2 test says little about the suitability of the continuum model for modelling the rock mass within the Aberg repository.

3.3 Comparison between the continuum model and alternative models

Major comments

An "Alternative Models Project" (AMP) was undertaken to compare predictions from the continuum model with results from two "alternative" (discrete-fracture-network and channel-network) models that do not rely on the same assumption. Due to the questionable validity of the continuum model for sparsely fractured crystalline rock, this comparison is crucial for confidence in the geosphere modeling. Hence the inclusion of such an exercise is to be applauded.

Unfortunately, the SR 97 main report series gives very few details about the Alternative Models Project. The importance of this comparison warrants a more clear description of the models and comparison of the results. Comments given below on the specific models are based on a supplementary review of the background reports by Dershowitz et al. (1999) and Gylling et al. (1998).

In the limited results that are presented in the the SR 97 Main Report, several discrepancies between the continuum model and the "alternative" models are apparent. These discrepancies (described in the detailed comments, below) weaken the argument that the effects of conceptual uncertainty regarding the continuum model are negligible.

The comparison between models was only made for the Aberg site. As Aberg is described as the most highly fractured of the three sites, it should be expected that the fractured rock here would behave more nearly as a continuum than at the other two sites. Generalization of the findings of the alternative models project to the Beberg and Ceberg sites has not been justified.

The comparison with the "alternative" models must furthermore be regarded as weak because significant sources of uncertainty in the "alternative" models were not considered. In particular, there appears to have been no effort to explore "pessimistic" cases of the "alternative" models. Evaluation of these uncertainties using variational cases could have led to larger discrepancies in the results.

Finally, the range of uncertainty explored by the combination of continuum and "alternative" models, when taken together, is limited because none of these models combined a strong, realistic description of rock mass heterogeneity with a strong, realistic description of fracture zone heterogeneity. Rather, it can be argued that contrasting descriptions of heterogeneity for the separate divisions of the geosphere tended to have offsetting results, leading to convergent rather than divergent predictions of safety parameters. This point is discussed in detail in the section, "Alternative Models Project."

To provide definitive support for the use of the stochastic continuum model in further safety calculations, a comparison needs to be made with alternative models that incorporate strong, realistic, models of both fracture zones and the rock mass.

Variational cases need to be considered for each alternative model, to ensure that an adequate appraisal has been made of global uncertainty.

Detailed comments

The Main Report [Vol. II, p. 259] states that all three types of models give consistent travel times and fluxes, particularly in terms of median values. This statement is arguable if one examines the few data that are presented in Figure 9-17 of the Main Report [Vol. II, p. 260]. This figure shows the medians, 5^{th} percentiles, and 95^{th} percentiles of the predicted distributions of t_w and q. Extreme values and standard deviations are not shown.

Figure 9-17a shows that the median travel time predicted by the DFN model is one half order of magnitude lower (faster) than that predicted by the continuum model. The CN model also predicts systematically faster travel times than the continuum model. The median travel time for the continuum model is nearly equal to the 95^{th} percentile of t_w for the DFN model, showing that nearly all of the transport paths in the DFN model are faster than the median transport path for the continuum model. To some extent this discrepancy can be explained by the exclusion of the 40% "nonconductive" canister positions that are mentioned in the text. However, this does not explain the similar discrepancy for the CN model (nor would the use of median particle travel times as suggested in the text, p. 259).

In Figure 9-17b the median groundwater flux at repository depth, as predicted by the discrete fracture model, appears to be 0.7 order of magnitude higher than that predicted by the stochastic continuum model. Again, the bulk of the q distribution for the DFN case lies to one side of the median value for the continuum model. The 95^{th} percentile value of q for the DFN model is about a factor of 5 higher than the corresponding statistic for the continuum model.

The distributions of both the CN and DFN predicted flux values are markedly asymmetrical on the log scale, in contrast to the continuum model results which are quite symmetrical. The non-Gaussian form of the CN and DFN results suggests that both of these models may have elongated tails in the direction of high fluxes, *i.e.* both models could tend to predict a small chance of canisters experiencing extreme fluxes, much higher than would be predicted with significant probability by the Gaussian stochastic continuum model.

The Main Report states that there were "relatively few" realizations for the discrete-fracture network model (10 realizations, according to Dershowitz et al., 1999), and hence the statistics are less reliable. Presumably the 5^{th} and 95^{th} percentile statistics would be most sensitive to the limited number of realizations. The Main Report also states that only a portion of the repository was represented in the discrete-fracture network model, so possibly the effects of spatial variability (with respect to release position) are underrepresented in this model relative to the other two models.

It is notable that the DFN model predicts higher extreme values of flux, despite the limited number of realizations and limited sample of spatial variability. Rather than dismissing these discrepancies as the results of a small sample, the possibility should be considered that even greater discrepancies might be evident if spatial and ensemble variability had been more thoroughly sampled.

The comparison between the continuum model and "alternative" models was made only for the Aberg site, which was the most highly fractured site, according to SKB's assessment. A site that is highly fractured, and hence farther from the percolation threshold, could be expected to show the closest similarity between continuum and discrete models. Greater discrepancies could be expected for the other two sites which are less fractured, and hence more likely to contain poorly percolating fracture networks. A few of the difficulties in dealing with poorly percolating networks are discussed in the example FEP description by Skagius et al. (1995, p. C-4).

The use of "alternative" models that attempt a more accurate representation of the physics of groundwater flow in fractured rock is commendable, but their application in SR 97 was very restricted. The results given in Figure 9-17 pertain to just one variant of each "alternative" model. Without some attempt to explore conceptual and data uncertainty within these alternative modeling approaches, the comparison between "alternative" models and the continuum model must be regarded as very weak.

For example, within the discrete-fracture network approach, a key conceptual uncertainty concerns the choice of a stochastic model for simulating fracture locations. A fracture-location model that tends to generate clusters of fractures with geometries similar to small-scale fracture zones (such as have been noted at the Aberg and Beberg sites) can produce very different flow and transport behavior than one that has the fractures more uniformly distributed. Other key data uncertainties such as the fracture length (size) distribution also need to be explored.

4. Alternative Models Project

In SR 97, an attempt was made to test whether the impact of the continuum assumption has a substantial impact on repository performance, by comparing the predictions of three types of models: (stochastic) continuum, discrete-fracture network (DFN), and channel-network (CN). The comparison was made in terms of predicted ranges of water "travel times" t_w, groundwater flux at repository depth, and "F factor.". This is described in Sections 9.8.4 and 9.9.7 of the Main Report.

Major comments

The continuum and "alternative" models differ in their treatment of heterogeneity in different portions of the bedrock: major fracture zones, smaller-scale fracture zones, and the "rock mass" that lies between these fracture zones.

None of the models explicitly considers the consequences of smaller-scale fracture zones, although the presence of these smaller-scale fracture zones was indicated by Saksa and Nummela (1998).

Based on the detailed review comments in the following sections, the treatment of heterogeneity in the rock mass and major fracture zones can be summarized for the three types of models as follows:

Type of model	*Rock mass heterogeneity*	*Fracture zone heterogeneity*
Stochastic continuum	Weak (optimistic)	Strong (most realistic)
Channel network	Weak (optimistic)	Intermediate
Discrete fracture network	Strong (most realistic)	Weak (most optimistic)

None of the models combined a strong (realistic) description of rock mass heterogeneity with a strong (realistic) description of fracture zone heterogeneity. Thus all three of the models were optimistic in some respect, in their overall treatment of heterogeneity.

Furthermore, it can be suspected that the contrasting descriptions of heterogeneity for the separate divisions of the geosphere had partly offsetting effects, leading to convergent predictions of safety parameters.

To provide definitive support for the use of the stochastic continuum model in further safety calculations, a comparison needs to be made with alternative models that incorporate strong (realistic) models of both fracture zones and the rock mass.

Variations of the alternative models should be used to assess the robustness of the predictions with respect to major aspects of uncertainty in the alternative models. In order to develop confidence in the stochastic continuum model as a tool for performance assessment, it must be shown that the idealizations inherent to this model do not prevent accurate assessment of significant sources of uncertainty. Thus the comparison of

models must go beyond a simple check of whether base-case versions give similar ranges of results.

4.1 Treatment of rock mass heterogeneity

Stochastic continuum model

The stochastic continuum model that was used as the main hydrologic model for SR 97 assumes that the rock mass can be modeled as a continuum in which hydraulic conductivity is a stochastic, spatially correlated process. In contrast with random network models such as discrete-fracture network models, this type of model assumes a very regularly connected system in which continuity of hydraulic head between adjacent blocks of the rock is assured, even if locally low values of hydraulic conductivity may result in restricted flow between adjacent blocks.

Spatial correlation of hydraulic conductivity values results in a possibility for the model to generate some moderately preferential flow paths due to clusters of relatively high-conductivity blocks. For the type of spatial correlation model that was used for most of the HYDRASTAR runs (isotropic covariance model), there is no tendency for higher-conductivity clusters to be elongated in any particular direction. An alternative model for spatial correlation (anisotropic covariance model) was considered as a variational case. This alternative model tends to produce higher-conductivity clusters that are elongated along a particular direction or within a particular set of parallel planes. However, even this type of continuum model is less likely to predict strongly preferential flow and transport pathways than a discrete network model. Hence the stochastic continuum model is a relatively weak (optimistic) model of rock mass heterogeneity.

Calculations of travel times and the *F* ratio from the continuum model are based on a single, uniform value of porosity and apparently a single, uniform value for flow wetted surface. As stated by Widén and Walker (1999, p. 55 and elsewhere), the calculated *F* ratio with this model is simply a [constant] multiple of the travel time. It would be more realistic to regard porosity and flow wetted surface as variable from place to place within the site. Neglecting this aspect of heterogeneity has likely led to a reduction in the predicted ranges of travel times and *F* (It should be noted that heterogeneity in effective porosity would not affect *F*, as it depends only on the ratio of advective velocity to the wetted surface per volume of water, or equivalently, the ratio of Darcy velocity to the wetted surface per volume of rock).

Discrete-fracture network model

The discrete fracture network model used in the alternative models project (Dershowitz et al., 1999) incorporates several aspects of rock mass heterogeneity, in particular irregular connectivity within the rock mass and variation in properties between different conductive elements (fractures) within the rock mass. This can be viewed as a relatively strong (realistic) model of rock mass heterogeneity, based upon experience from sparsely fractured granitic sites such as Stripa, where anomalous transport paths and high variability of hydraulic head from point to point in the rock mass have been observed.

In this specific application of the discrete-fracture network model, only a single type of model for the fracture location stochastic process (the "BART" model) was used. This model reproduces certain observed aspects of the fracture system, namely the percentage of fractures that terminate at intersections with other fractures. However, the model does not necessarily reproduce the degree of structure in the fracture population that is suggested by other fracture location models (e.g. fractal or nearest-neighbor point field models) that have previously been derived for this site (Axelsson et al., 1989; Geier and Thomas, 1996).

The assessment that the BART model was "applicable" is described as having been based on an analysis of data from a relatively small area of the site, the TRUE-1 area (Dershowitz et al., 1999, p. 32). There is no indication that alternative fracture-location models such as fractal or nearest-neighbor models were found to be inapplicable. Without consideration of alternative fracture-location models, the degree to which this aspect of model uncertainty affects the predictions cannot be assessed.

The specific model as implemented did not represent heterogeneity or channeling within fracture planes, although this is possible to do within the DFN approach (e.g. Nordqvist et al., 1995). The model assumes that there is no correlation of hydraulic or transport properties between the different fractures that connect to form a given flow path. It also assumes, apparently, that there is no correlation between fracture hydrologic properties and fracture geometric properties such as size. In these respects the model could be regarded as optimistic.

In calculating radionuclide retention properties, the model assumes that the entire surface area of each fracture segment (strictly, the area between intersections with other fractures where inflow and outflow occur) is available for sorption and matrix diffusion. In other words, access to the rock is not reduced by channelization due to aperture variations, such as are ordinarily present in natural fractures. This is also an optimistic assumption.

Channel network model

The channel network model (Gylling et al., 1999) does not account for irregular connectivity in the rock mass, as the channels are connected in a regular 3-D grid. In this respect the model is similar to a continuum model. Simulations based on a regularly connected model are less likely to yield anomalous connections than a model such as the DFN model, in which not only the hydraulic properties, but also the geometric configuration of the conductive features (fractures or channels) is treated as being random. On this basis the channel network model should be regarded as a weaker (more optimistic) model of rock mass heterogeneity than the DFN model.

Flow and transport properties are assumed to vary between channel segments, e.g. according to a lognormal distribution for channel conductance. An implicit assumption, apparently, is that there is no correlation of properties between adjacent channels. In this respect, the model of rock mass heterogeneity is weaker (more optimistic) than the stochastic continuum model, in which hydraulic conductivity is considered to be spatially

correlated, so that there is a somewhat greater chance of producing extended pathways of relatively high K. On the other hand, the conductances of channels that emanate in different directions from a given grid node are also uncorrelated, which means that the channel model incorporates a degree of random anisotropy on the scale of the grid spacing.

The formulation of the channel network model includes a parameter for channel length L, which is the regarded as the physical distance (possibly tortuous) along a channel between a given pair of nodes nodes that are adjacent to each other in the grid. The conceptualization apparently allows for L to be a random variable, in which case the regular 3-D grid used for calculations would represent a deformed version of the assumed physical grid. However, in the report by (Gylling et al. 1999), I could not find any statement of a probability distribution that was used for L; from this I presume that a single value was used uniformly throughout the model.

A major difference with the continuum model is that, in the channel-network model, mixing of solute carried along different streamlines is restricted to occur only at the channel intersections (grid nodes). Transport simulations based on this model would result in different macrodispersion properties than in a corresponding continuum model. However, in the present study it appears that the CN model was used only to calculate properties of single streamtubes representing a number of channel segments in series, rather than all of the channel segments that would carry part of a solute plume. This is implicit in the formulae for calculating the variables $t_{tot,i}$, $F_{tot,i}$, and $a_{w,i}$ and in statements about the use of CHAN3D to produce data for FARF31 (Gylling et al., 1999, p. 17-8). Thus this distinction between the channel-network approach and the continuum approach plays no role in the alternative models project.

The channel network model does explicitly embody an assumption that flow and transport occur through distinct channels that would expose radionuclides to only a fraction of the rock mass. The assumption of channelized flow in fractures is considered to be realistic in view of in situ studies such as the Stripa Project (Abelin et al., 1990). However, for the type of calculations that were performed in the AMP, it is not clear that this conceptualization has any consequence beyond what would result from a finite-difference continuum model in which hydraulic conductivity is randomly anisotropic, and where the tracing of streamlines is constrained to follow the orthogonal grid that connects the centers of the blocks in the continuum model.

The model as applied in this project assumes that all channel segments in the rock mass have a uniform value of flow wetted surface FWS (Gylling et al., p. 16), which is taken to be 10% of the FWS that is estimated based on the total conductive fracture frequency of the fracture zones. Thus no attempt was made to estimate this value for the rock mass as distinguished from the fracture zones. The basis for choosing this 10% factor is not stated. If this corresponds to the average contrast in fracture frequency between rock mass and fracture zones, it should be regarded as an optimistic value. If the rock mass is close to the percolation threshold, it should be expected to have reduced connectivity

relative to the fracture zone rock, and hence a lesser fraction of the conductive fracture frequency will actually be exposed to radionuclides along transport paths.

This estimate of FWS is furthermore estimated as an average property for each major division of the rock (either the entire rock mass or all of the fracture zones) at the site. Thus it does not account for heterogeneity of FWS within these major divisions, which would seem to be more realistic. For example, if the Aberg site contains minor fracture zones (as suggested in the structural-model review by Saksa and Nummela, 1998), "channels" within these features would be more closely spaced (have a smaller spacing H, in the notation of Gylling et al., 1999, p.13) and thus higher-than-average values of a_R, while "channels" in the intervening rock mass would have lower-than-average values of a_R. A distribution of a_R values would be more realistic, and would presumably result in a wider predicted range of the critical parameter F.

Summary of treatment of rock mass heterogeneity

Three fundamentally different conceptual assumptions were used for the spatial structure of rock mass hydrologic properties, in the three different types of models:

SC model: **regularly connected,** spatially correlated**,** isotropic hydraulic conductivity
CN model: **regularly connected,** spatially uncorrelated, randomly anisotropic conductances.
DFN model: **irregularly connected**, spatially uncorrelated, random fracture transmissivities.

The irregular connectivity of the DFN model would be expected to produce the highest degree of flow and transport localization within the rock mass. The channel network and continuum models are similar in their use of a regularly connected flow grid, but differ in the local representation of conductivity in the rock mass. Both the channel network and continuum models should be regarded as optimistic in their representation of rock mass heterogeneity, due to their regular connectivity and the relatively weak representation of spatial structure in the hydraulic conductivity or channel conductance field. All three of the models incorporate various assumptions which could be regarded as optimistic, in the calculation of retention parameters.

4.2 Treatment of small-scale fracture zones

The SR 97 Data Report (p. 54) cites the structural-model review by Saksa and Nummela (1998), which noted that fracture zones in the size range 10 m - 1000 m have only been "partly" considered for Aberg, and have not been included at all in the structural models for Beberg and Ceberg. Small-scale fracture zones are of concern especially if they tend to be connected to major fracture zones, e.g. for reasons related to fracture zone genesis and reactivation.

The main hydrogeologic models that were used in the performance assessment do not explicitly account for small-scale fracture zones in a deterministic sense. These models, based on the concept of a stochastic continuum, arguably do not permit resolution of high-conductivity fracture zones on a scale less than about 5 block dimensions. The smallest block scale that was found to be practical in this study was 25 m, which implies that fracture zones with length scales less than about 125 m could not be resolved.

Moreover, it is arguable whether a geostatistical analysis based on regularized (effectively, smoothed) data for effective hydraulic conductivity will yield a covariance function that adequately reproduces discrete, high-K structures on a scale similar to the small-scale fracture zones. Use of Gaussian as opposed to non-Gaussian (e.g. indicator variable) simulations may also limit the resolution of "fracture-zone-like" features that these models can produce. Thus it is doubtful whether this type of hydrogeologic model can represent the small-scale fracture zones in a stochastic sense.

An attempt was made to simulate a more structured K field by use of anisotropic covariance functions (Walker and Gylling 1998). This as done in an attempt to mimic an interpreted, overall anisotropy in rock mass K, not to mimic observed patterns of second-order fracture zones. In any case this approach would only tend to reproduce a single set of similarly-oriented, high-K and low-K pseudoplanar structures, not multiple sets such as are observed at these sites (e.g. Tirén et al., 1996).

The discrete-fracture network (DFN) models used as part of the "alternative model project" is capable of stochastic simulation of small-scale fracture zones. Examples of fracture location models that tend to produce stochastic, fracture-zone-like clustering of fractures are the fractal-based (Levy-Lee) and compound Poisson process (nearest neighbor) fracture location models, which were found to be applicable for the Aberg and Beberg sites based on past DFN analyses (Axelsson et al., 1989; Geier et al., 1992; Geier and Thomas, 1996). The specific type of DFN model that was used in the alternative model project, the BART model, is not designed to reproduce strong clustering as in second-order fracture zones, but only to mimic connectivity statistics in a statistically homogeneous fracture population.

The channel-network model does not explicitly consider small-scale fracture zones. The channels in the rock mass portion of the model could perhaps be viewed as representing flow channels in small-scale fracture zones as well as in the remainder of the rock mass.

However, the rock mass domain is modeled as a single, statistically homogeneous population of channels.

4.3 Treatment of heterogeneity in major fracture zones

The treatment of the major, "deterministic" fracture zones in the discrete fracture network model was qualitatively different from that in the channel network and continuum models. The continuum model (Widén and Walker, 1999) assumes that the major fracture zones ("conductor domain") are heterogeneous, with the same geostatistical properties as the rock mass except that the mean log hydraulic conductivity is shifted by a specified amount. In the channel network model (Gylling et al., 1999), the channels within major fracture zones were assigned independent random values of K from a lognormal distribution with median K related to median estimate of fracture zone transmissivity. In the discrete fracture network model, the large-scale, planar features representing major fracture zones were apparently assigned single values of transmissivity (Dershowitz et al., 1999, Table 4-4), and thus were modeled as homogeneous features.

Thus three fundamentally different conceptual assumptions were used for the spatial structure of major fracture zone hydrologic properties, in the three different types of models:

continuum:	3-D **heterogeneous,** spatially **correlated** hydraulic conductivity
channel network:	3-D **heterogeneous,** spatially **uncorrelated** hydraulic conductivity.
discrete-fracture network:	2-D **homogeneous** transmissivity.

The spatially correlated, heterogeneous model for fracture zone properties, as used in the continuum model, would be expected to produce the highest degree of flow and transport localization within the major fracture zones. The uncorrelated, but still heterogeneous model, as used in the channel network model, would give a lesser degree of localization. The discrete fracture network model did not include a representation of heterogeneity in the major fracture zones, and hence would tend to yield the lowest degree of flow and transport localization within the zones.

Past geostatistical analysis of the Aberg data by Tsang (1996) showed that the possibility of long-range spatial correlation of hydraulic conductivity within the major fracture zones cannot be excluded. Past hydrologic modeling of the Aberg site using a discrete-feature model similar to the discrete-fracture network model (Geier, 1996) showed that spatially correlated heterogeneity within the major fracture zones is potentially a significant source of variation in groundwater travel times and radionuclide retention properties, **in addition to** the effects of rock mass heterogeneity as represented by a discrete-fracture network model.

5. Radionuclide transport and retention

Major comments

The SR 97 conceptual model of radionuclide transport is based on a 1-D streamtube formulation (as embodied in the numerical model FARF31). A key parameter that emerges with this formulation is the parameter F , which is variously referred to as the "F ratio," "F factor," etc.

The 3-D stochastic continuum and "alternative" models were not used directly for modeling solute transport. They were used only to predict F values and discharge points for streamtubes passing through the repository. These predictions were made on the basis of flow simulations and various forms of flow path tracing (streamline tracing or weighted graph searches) in combination with geometric assumptions regarding the flow wetted surface along segments of flow paths.

The fact that the 3-D models were not used for actual transport simulations means that certain distinctive characteristics of the "alternative" (DFN and CN) models, such as mixing at intersections of branches in the network and consequent macrodispersion effects, did not play any role in the predictions. While this might not be of direct, major significance for predicting radionuclide retention, it influences the comparison of models. It should be clearly understood that the comparison between models is solely on the basis of flow path characteristics, not transport predictions. Effects of flow field complexity on radionuclide transport have not really been explored in SR 97.

The similar predictions of F values (especially 5^{th} percentile values, which are of greatest interest for safety assessment) between models appears to be partly due to a limited range of assumptions regarding flow wetted surface. All models are based essentially on geometric estimates of flow wetted surface that are based on the frequency of conductive intervals in detailed (hydrologic) packer testing, along with an assumption that the entire area of each fracture or channel is equally accessible to radionuclides.

Separate estimates of F given on p. 277 of the SR 97 Main Report (Volume II) are discussed as if they were independent estimates, when they are not. This gives a misleading impression of uncertainty regarding this crucial parameter. As is the case with the comparison of alternative models, the problem is that all estimates of this parameter essentially are derived from the same conductive-interval frequency data and similar geometric assumptions regarding the accessibility of fracture/channel surface area to radionuclides.

Due to the importance of this parameter, more independent methods are needed for estimating F and the related parameter, flow wetted surface.

Elaboration of major comments

Separate estimates of *F* given on p. 277 of the SR 97 Main Report (Volume II) are discussed as if they were independent estimates, when they are not. To present these as independent estimates of *F* is misleading. The "reasonable value" of a_w (wetted surface per unit mobile water volume) of 10^3 m^{-1} appears to have been obtained directly by dividing the "reasonable value" of a_r (wetted surface per unit rock volume) of 1 m^{-1} by the "reasonable" flow porosity of 10^{-3}. (SR 97 Data Report, pp. 90-94). The "reasonable" values of the parameters t_w and q are of course closely related for a given assumed flow porosity and travel distance, as illustrated by the equation on p. 257 of the Main Report, Volume II (noting that Ki is an estimate of q, where K is representative hydraulic conductivity and i is the average hydraulic gradient).

F ratio comparison in the Alternative Models Project

A comparison of these models in terms of the "*F* factor," which is a critical parameter for FARF31 calculations, is given in Table 7.3.3 of the SR 97 Data Report. The Main Report [Vol. II, p. 278-279] states that "*F* factors calculated with the continuum model and the discrete network model are, however, relatively similar." In Table 7.3.3, the medians and 5^{th} percentile statistics for F are indeed quite similar among the three types of models, although the reported spread of values for the DFN model exceeds that for the base-case continuum model by 1.2 orders of magnitude. The Data Report mentions [p. 93] that the total spread of *F* values calculated by the DFN model is as much as 2 orders of magnitude wider than the other models.

In the discussion of *F* ranges predicted by alternative models, on p. 93 of the Data Report, in two places there are statements to the effect that the alternative model predictions, particularly the DFN results, "are not full comparable" due to differences in estimation technique. These statements are confusing, considering that in the introduction sections of two of the AMP reports (Widén and Walker, 1999; Dershowitz et al., 1999) it is stated that, "[t]he emphasis of the AMP is that the results of the three approaches should be as comparable as possible."

As *F* is a crucial parameter in prediction of rock barrier performance, and as one stated goal of the AMP is "to illustrate rock barrier performance using different conceptual models…" (Widén and Walker, 1999; Gylling et al., 1999; Dershowitz et al., 1999), it is of great interest to know whether the different estimation techniques lead to different ranges of *F*. When differences emerge from the comparison of alternative models, the reasons and implications should be explored and discussed.

The 5^{th} percentile statistics for *F* (which are the most critical as the lowest values imply the maximum peak release to the biosphere) agree for all three types of models, within a factor of 1.3. This is remarkable for a parameter that ranges over 4 orders of magnitude. It should be considered whether these estimates are truly independent, or whether there is some shared set of assumptions behind the calculations that lead to these as limiting values.

Both the SC and CN models used uniform values of the flow porosity ε_f. Both the SC and CN models used values of flow-wetted surface a_R based directly on estimates of the average conductive-fracture frequency at the site, which in turn were based directly on the percentage of conductive sections in packer tests. In the SC model, a single value (1.23 m^{-1}) is assumed to apply for the entire site. In the CN model, a nearly identical value is used for fracture zones (1.2 m^{-1}), while a lower value (0.12 m^{-1}) is assumed to apply for the rock mass. Neither model considers variability of this parameter within the rock mass or within fracture zones.

As for flow parameters, the alternative-model calculations ought to be carried out for for a representative range of alternative-model variants, to ensure that conceptual and data uncertainty in these approaches is also accounted for in the evaluation of global uncertainty.

In the Table 7.3.3 [Data Report], it is notable that the 5^{th} percentile value for F obtained by SKI in the SITE-94 study of Äspö was a full order of magnitude lower than any estimate obtained in SR 97. A value very close to this low estimate was adopted as a "pessimistic" value for Aberg in SR 97. Significantly higher values of F were chosen as "pessimistic" values for the Beberg and Ceberg sites, where there was no independent estimate. This appears to have been a coincidence, but suggests that there may be a risk of underestimating the possible range of this critical parameter, if the analysis is limited to a few teams that are working from a shared set of conceptual assumptions.

Flow porosity

The main modeling approach used a uniform value of flow porosity to calculate groundwater advective travel times t_w. The value of 10^{-4} that was used is described as "pessimistic" (SR 97 Main Report, p. 257). This appears to be based on the argument given on p. 91 of the Data Report, where it is stated that tracer tests from Aberg and Beberg suggested a median flow porosity of 10^{-3}.

As the tracer tests at both Aberg and Beberg have been carried out dominantly within fracture zones, the porosity estimates from these tests should be interpreted as representative of fracture zone flow porosity. As noted on p. 91 of the data report, the range of estimates from these tests is moreover large, and reflects spatial variability. It is also noted here that "there are indications" that different values of flow porosity may apply for different parts of the rock. However, the Data Report asserts that "more precise parameter estimates would be needed to further substantiate such a conclusion before it could be considered in performance assessment."

If there are indications from the site interpretation that flow porosity is variable between rock units, the question needs to be asked as to whether the use of a single, uniform porosity value is more defensible than the use of variable porosity values. The Data Report states that there is "no clear experimental support" for assigning variable values of flow porosity, but from what has been stated above we can also infer that there is no clear

experimental support for using a single, uniform value of flow porosity. The Data Report does mention practical problems that would arise from the use of a variable flow porosity, with the far-field radionuclide transport code FARF31.

6. Repository system description

System Description using THMC diagrams

In the THMC charts, some of the "variables" for the geosphere are very broadly defined. A better term would be "lumped variables" or "variable categories." The goal in defining such broad categories is apparently to keep the THMC charts manageable in size and easy to read. However, there is a risk that such broad categories may tend to obscure interactions between processes and the actual geosphere variables that make up these variable categories.

For instance, combining all geosphere "cavities" from fracture zones to micropores, as well as the EDZ etc., under the variable category "fracture geometry" is counterintuitive, and can easily lead to overly broad statements about the influence of specific processes. Fracture zones are not simply "cavities" or "collections of cavities," they are zones of relatively intensely fractured rock that commonly have hydrologic, mechanical, and mineralogical characteristics distinct from the surrounding rock, stemming from past episodes of tectonic and hydrothermal activity. The response of fracture zones to processes such as seismicity associated with deglaciation can be expected to differ qualitatively from the response of micropores in the rock matrix. Micropores, on the other hand, are pervasive both within fracture zones and within the less fractured "rock mass." It is not realistic to speak, say, of the response of the rock matrix to stress without incorporating the influence of the micropores on the elastic properties of the rock.

The chief hazard with this lumped approach is that interactions between more specific entities and processes may be overlooked. Considering the example of "fracture geometry" it seems possible that an interaction might be assessed with simple, macroscopic fractures in mind, but neglecting fracture zones or microfractures and pores. To guard against this, an additional level of interaction assessment may be needed to ensure that interactions are properly assessed for all of the entities/processes that have been lumped together as a single "variable."

7. Details of Repository Design

Repository Layout

The repository layouts do not show the locations of any of the access tunnels, access ramps, or ventilation shafts (if required). The performance assessment ought to be based on consideration of a complete repository layout. Access tunnels will presumably need to pass through the major fracture zones, and presumably special sealing/plugging procedures will be called for in these locations. According to Section 3.5.2 of the Repository System Report (p. 25), "SR 97 does not include the analysis of permanent plugs." In the absence of any justification for neglecting this aspect of the repository system, this must be regarded as a gap in the performance assessment.

The lower level of the Aberg repository (Figure 6-3b) includes a single tunnel (red line) in a very narrow block (gray band) that appears to be less than 20 m wide after allowing for the respect distances to the neighboring major fracture zones. It is not clear whether the definition of "respect distances" that is used in defining these blocks takes account of uncertainties regarding fracture zone location, planarity, and thickness (See comments on "Section 5.2.3 Respect distance" in the Repository System Report). If it does not, then the reasonableness of placing a tunnel at this location is questionable. Minor deviations in fracture zone thickness or nonplanarity would result in violation of the specified "respect distances."

This issue hinges upon SKB's interpretation of the concept of "respect distance;" *i.e.* whether this is to be regarded as a firm criterion that is relied upon in the performance assessment, or simply an ad hoc rule that is used in the early stages of design. A more clear statement of the role of this concept in performance assessment would be helpful.

A second, and perhaps more significant concern with this deposition tunnel stems from the likelihood that two subparallel, major fracture zones such as these are likely to be structurally related. This implies that there is a high likelihood of encountering multiple, second-order fracture zones spanning the tabular "block" between these major fracture zones. An analogue would be the "block" between the upper and lower conductive zones within Zone 2 at Finnsjön, which has been interpreted as part of a compound fracture zone with multiple step-over zones. Second-order fracture zones that connect directly to major fracture zones may be more significant for performance than has been recognized in this assessment (see comments on "Treatment of second-order fracture zones").

Factors for utilizing deposition positions

In Section 3.1.5 of the Repository System Report, several of the factors for considering whether canister position can be utilized are directly observable or measurable (e.g. inflow of water). Others such as stability and probability of tectonic impact would presumably require rock mechanical calculations.

It would be preferable to express the design criteria in terms of the directly observable data that are needed (e.g. rock friction angle, fracture orientations relative to principal stresses). Otherwise this list of criteria needs to be accompanied by further explanation of the methods for rock mechanical analysis.

Shaft boring of deposition holes

The Repository System Report [Section 3.2.2, p.18, last paragraph] states, "The conclusions drawn thus far are that a small zone is formed near the rock wall during shaft boring that *may* have elevated hydraulic conductivity in the axial direction of the deposition hole. *This is advantageous for water saturation of the buffer, since an even distribution of water along the entire deposition hole is thereby achieved* …" (emphasis added).

Has this last point actually been demonstrated, or is this speculative? Increased hydraulic conductivity (K) as described can perhaps be expected to produce a *more even* distribution of water along the deposition hole, but the degree to which this can be expected to take place does not appear to have been established, either by physical demonstration or by modeling.

A small increase in K adjacent to a deposition hole might not be sufficient to achieve "an even distribution of water along the entire deposition hole." If the boring-induced K is small relative to the transmissivity of a water-bearing fracture intersecting the borehole, an uneven distribution of water and hence uneven saturation of the bentonite buffer might still occur.

The conclusion appears to be based on references to work that characterized (1) the extent of fractures formed by indentors such as on a shaft boring machine, and (2) porosity changes adjacent to experimentally bored tunnels and deposition holes. Neither fracture extent nor porosity relates directly to hydraulic conductivity, although a positive correlation with these is certainly to be expected.

The authors need much stronger evidence to support their assertion that "an even distribution of water along the entire deposition hole is thereby achieved."

Grouting

[Repository System Report, Section 3.2.4, p. 19] Possible effects of grouting on the natural hydrologic system are not mentioned here. Areas of concern include (1) alterations in natural fracture flow paths due to incomplete sealing of the fractures, e.g. causing increased advective velocities through a subset of the fractures, and (2) dissolution and reprecipitation of grout components.

Permanent plugs

[Repository System Report, Section 3.5.2, p.25] The discussion of backfill settling is out of place. This problem presumably could occur with or without the presence of rigid plugs, although it will be accentuated in the vicinity of rigid plugs that resist tunnel closure. Even without rigid plugs, cavities could form in backfill with inadequate compaction and/or inadequate swelling properties, if there is a high contrast in elastic moduli between the bedrock (e.g. granite) and the backfill (e.g. crushed rock mixed with bentonite). This also relates to the tunnel stabilization criterion mentioned in 3.4.3 under the heading "Backfill."

Plugging of boreholes

[Repository System Report, Section 3.5.2, p. 25] There is an inconsistency here betweeen the description of the method for sealing boreholes by inserting "perforated copper pipes filled with compacted bentonite," and the discussion of hole pretreatment by cementing and redrilling prior to feeding down "the concrete fill." Should the latter phrase in quotes be "the bentonite fill" ? References to the relevant studies could help to clarify.

In stating the safety case, it ought to be clear as to whether the selected borehole-plugging method has been shown to be completely effective (i.e. resulting in a nearly equal or lower conductance along the borehole than the bedrock that has been drilled out).

If borehole plugging is not completely effective in this sense, the predicted hydrologic properties of the borehole plugs (hydraulic conductivity, flow porosity, wetted surface) ought to be described in quantitative terms, so that the potential for these to act as preferential transport paths can be assessed. It seems reasonable that a high specific wetted surface area in the borehole plugging material could prevent the release of hazardous concentrations of sorbing radionuclides, even if the plugged boreholes act as preferential conduits for groundwater movement. However, this ought to be demonstrated or at least discussed in the safety case.

The report states specifically that "boreholes connected to the ground surface" are to be sealed. It does not state whether the same sealing methods will be used to seal boreholes (e.g. probe holes) that may conect from repository tunnels to hydrologic features such as fracture zones that may provide paths for rapid transport to the surface. If this is assumed to be part of the repository design, it ought to be stated as part of the safety case.

The description of the pretreatment procedure for boreholes in discontinuities or poor rock raises the question as to whether borehole deviation during redrilling through cemented sections might result in abandonment of unsealed sections of borehole, or strongly elliptical sections in which the plug (e.g. perforated copper tube) fills only part of the hole's cross section. This issue might possibly be resolved by a more clear description of the methods that SKB intends to use, and by a more complete description of the borehole sealing studies that are mentioned here without references.

Have the borehole sealing procedures, including cementing and redrilling, been demonstrated for very long boreholes drilled from the surface, where problems of borehole deviation could be expected to be more severe? Have these procedures been demonstrated for poor quality rock and/or wellbore breakout conditions?

Retrieval of deposited canisters

[Repository System Report, Section 3.5] As retrievability of canisters is a design goal for the SR 97 hypothetical repositories, this must impose constraints on the choices of materials, e.g. using bentonite/crushed rock rather than cement to backfill tunnels. Factors affecting retrievability should be mentioned as design criteria.

8. Site Descriptions

Geological description

[Repository System Report, Section 4.3.1 Aberg, under heading Local scale, 4th paragraph on p. 36] "The length of fractures is measured in outcrops and on tunnel walls and is independent of rock type."

This is debatable. Trace length distributions for greenstone and aplite/fine-grained granite (from the Äspö pre-investigation stage) differed significantly from those for Äspö granodiorite and Småland granite, according to analysis by Geier and Thomas (1996). Moreover, censoring effects due to sampling on cleaned trenches and tunnel walls of restricted width (2-3 m) may obscure differences in the tails of the trace-length distributions, which represent the longest fractures. If this statement is based on a statistical comparison of the fracture data, a citation would be helpful.

[Section 4.3.3 Ceberg, uder the heading "Regional scale", subheading "Fracture zones and fractures"] "Despite the fact that several boreholes intersect these zones, their geological and hydraulic properties should be regarded as uncertain."

The same could be said for most, if not all of the fracture zones at Aberg and Beberg. Why is this statement given for Ceberg and not the other sites? Why are no variability or uncertainty estimates given in the tables of fracture-zone transmissivity or hydraulic conductivity values for the other sites? Would it be better to say that the uncertainty of the Ceberg estimates should be regarded as high relative to the equivalent estimates for the other sites?

From the few cases where multiple boreholes penetrate single fracture zones at Äspö and at Finnsjön, it is clear that fracture zone widths and interpreted point transmissivities vary between boreholes, sometimes by orders of magnitude.

Respect distance

[Repository Sytem Report, Section 5.2.3] The concept of a "respect distance" is defined here as: "*the distance from an interpreted discontinuity that is required to ensure that requirements on long-term safety for a canister position are met*."

Comment 1: It is not clear whether this definition takes into account uncertainty regarding fracture zone location, planarity, and thickness.

From structural geologic considerations it is probable that many fracture zones deviate substantially from tabular ("planar") form, and vary substantially in thickness. Detailed investigations of individual fault zones and fracture zones, e.g. the Fracture Zone Project at Finnsjön, confirm that this is the case. This situation is acknowledged elsewhere in the SR 97 report series. It is also acknowledged that fracture intensity in the rock mass often

tends to decrease with distance from fracture zones, which implies that the boundaries of fracture zones may be diffuse rather than discrete.

SKB should clarify whether "respect distance" is supposed to be sufficient to account for these types of uncertainty regarding the location of a fracture zone's boundaries, or whether it merely represents the minimum allowable distance to a fracture zone's actual boundary (assuming that this is accurately defined). If the former, we should expect that "respect distances" may need to increase e.g. with depth or distance from the nearest boreholes or tunnels where the fracture-zone boundaries have been determined, as uncertainty regarding fracture zone location (including uncertainty associated with geophysical measurements) generally increases with distance from the nearest points where data are obtained.

Comment 2: It is not clear how "respect distances" can be quantified a priori, based on the above definition. It is not clear what are the "requirements on long-term safety for a canister position" that have been used to establish respect distances for different categories of fracture zones, or how SKB has assessed the adequacy of a given respect distance for any given class of fracture zones. Are the specified "respect distances" based on generic modeling studies of radionuclide transport? If these are simply *ad hoc* rules to guide the preliminary stages of repository design process, based on subjective expert opinion, this should be stated more directly.

It might be reasonable to state that the adequacy of a given "respect distance" can only be judged by more elaborate, model-based assessments than would be practical at an early stage of repository design.

Effects of seismicity

[Processes Report, p. 188, last paragraph] "… this aspect of earthquakes [changes in fracture structure and resulting conductivity distribution] is not addressed in SR 97. … The mechanical effects on the repository are thus deemed to be more important than mechanical or hydraulic/hydrological effects on the geosphere."

It appears that the word "thus" here is inappropriate. Rather, the possible mechanical and hydrologic effects on the geosphere were simply not addressed, apparently because these were deemed to be of lesser importance. Further discussion of the grounds for this decision would be advisable.

9. References

Abelin, H., Birgersson, L., Widén, H., Ågren, T., Moreno, L., and Neretnieks, I., Channeling experiment. Stripa Project Technical Report 90-13, Swedish Nuclear Fuel and Waste Management Co., Stockholm, 1990.

Axelsson C-L., Jonsson, E-K., Geier, J.E., and Dershowitz, W.S., Äspo Hard Rock Laboratory discrete fracture modelling, SKB HRL Progress Report 25-89-21, Swedish Nuclear Fuel and Waste Management Co., Stockholm, 1989.

Dershowitz, B., Eiben, T., Follin, S., and Andersson, J., SR 97 – Alternative Models Project. Discrete fracture network modelling for performance assessement of Aberg. SKB Rapport R-99-43, Swedish Nuclear Fuel and Waste Management Co., Stockholm, 1999.

Geier, J.E. (SITE-94) Discrete-feature modelling of the Äspö site: 2. Development of the integrated site-scale model. SKI Report 96:6, Swedish Nuclear Power Inspectorate, Stockholm, 1996

Geier, J.E. (SITE-94) Discrete-feature modelling of the Äspö site: 3. Predictions of hydrogeological parameters for performance assessment. SKI Report 96:7, Swedish Nuclear Power Inspectorate, Stockholm, 1996

Geier, J.E., Axelsson, C-L., Hässler, L., and Benabderrahmane, A., Discrete fracture modeling of the Finnsjön rock mass: Phase 2. SKB Technical Report 92-07,Swedish Nuclear Fuel and Waste Management Co., Stockholm, 1992

Geier, J.E. and Thomas, A.L., (SITE-94) Discrete-feature modelling of the Äspö site: 1. Discrete fracture network models for the repository scale. SKI Report 96:5, Swedish Nuclear Power Inspectorate, Stockholm, 1996

Gylling, B., Moreno, L., and Neretnieks, I. SR 97 – Alternative Models Project. Channel network modelling of Aberg. Performance assessement using CHAN3D .SKB Rapport R-99-44, Swedish Nuclear Fuel and Waste Management Co., Stockholm, 1999

Long, J.C.S., Remer, J.S., Wilson, C.R., and Witherspoon, P.A., Porous media equivalents for networks of discontinuous fractures. *Water Resources Research*, Vol. 18, p. 645-658, 1982

National Research Council, *Rock Fractures and Fluid Flow – Contemporary Understanding and Applications*, National Academy Press, Washington, D.C., 1996.

Nordqvist, W., Dverstorp, B., and Andersson, J., On the specific surface area parameter: a sensitivity study with a discrete-fracture network model (SITE-94), SKI Report 95:30, Swedish Nuclear Power Inspectorate, Stockholm, 1995

Saksa, P. and Nummela, J., Geological-structural models used in SR 97. Uncertainty analysis. SKB Technical Report 98-12, Swedish Nuclear Fuel and Waste Management Co., Stockholm, 1998.

Skagius, K., Ström, A., and Wiborgh, M., The use of interaction matrices for identification, structuring, and ranking of FEPs in a repository system. Application on the far-field of a deep geological repository for spent fuel. SKB Technical Report 95-22, Swedish Nuclear Fuel and Waste Management Co., Stockholm, 1995.

SKB 1999. SR 97: Post-closure safety. Main report. SKB Report 99-06, Volumes I and II, Swedish Nuclear Fuel and Waste Management Co., Stockholm, 1999.

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

SR-97 – Waste, repository design and sites. SKB Technical Report TR-99-08, Swedish Nuclear Fuel and Waste Management Co., Stockholm, 1999.

SR-97 – Data and data uncertainties. SKB Technical Report TR-99-09, Swedish Nuclear Fuel and Waste Management Co., Stockholm, 1999.

Tirén, S., Beckholmen, M., Voss, C., and Askling, P., (SITE-94) Development of a geological and structural model of Äspö, southeastern Sweden. SKI Report 96:16, Swedish Nuclear Power Inspectorate, Stockholm, 1996. 1996

Tsang, Y.W., (SITE-94) Stochastic continuum hydrological model of Äspö. SKI Report 96:9, Swedish Nuclear Power Inspectorate, Stockholm, 1996.

Walker, D., Eriksson, L., and Lovius, L., Analysis of the Äspö LPT2 pumping test via simulation and invere modelling with HYDRASTAR. SKB Technical Report 96-23, Swedish Nuclear Fuel and Waste Management Co., Stockholm, 1996.

Walker, D., and Gylling, B., Site-scale groundwater flow modelling of Aberg. SKB Technical Report TR-98-23, Swedish Nuclear Fuel and Waste Management Co., Stockholm, 1998

Widén, H., and Walker, D. SR 97 – Alternative Models Project. Stochastic continuum modelling of Aberg. SKB Rapport R-99-42, Swedish Nuclear Fuel and Waste Management Co., Stockholm, 1999.

Appendix 1: Technical Background of the Author

Joel Geier is a Ph.D. candidate in the Geosciences Department of Oregon State University, presently completing a Ph.D. dissertation on groundwater flow and radionuclide transport in fault zones in granitic rock. Since 1987 he has been involved in research related to groundwater flow and radionuclide transport in fractured crystalline rock, as a senior engineer/hydrogeologist with Golder Associates and subsequently as a private consultant.

Past responsibilities have included development of the FracMan discrete-fracture network modeling code, revision and verification of the geostatistical code INFERENS for inference of stochastic-continuum model parameters, plus well test interpretation and modeling of flow and transport through fractured granitic rock at the Stripa, Finnsjön, and Äspö sites. As part of the SKI SITE-94 performance assessment study, he was responsible for evaluation of geosphere retention parameters based on discrete-feature modeling of groundwater flow and advective-dispersive transport from a hypothetical repository at the Äspö site, and also participated in the simple evaluation of geologic barrier potential, formulation of calculation cases for near-field and far-field PA codes, and documentation of site-specific data usage.

Review of SR 97 Performance Assessment

Pierre D. Glynn

U.S.Geological Survey
Water Resources Division
432 National Center
Reston, Virginia 22092, USA

This review is an independent technical evaluation of SR 97 by P.D. Glynn. It was carried out in response to a request of SKI as a part of ongoing technical and research cooperation between USGS and SKI. This review is not an official USGS statement on SR 97 or on any of the topics mentioned herein.

Introduction

My review focused on a careful reading of the English version of the main SR 97 reports with occasional referencing to supporting documents. I highlight here what I believe to be the most important questions and issues. Overall, SKB should be commended for obtaining a highly significant amount of scientific information concerning issues of relevance to nuclear waste disposal. In general, SKB's data collection efforts have been quite successful and SKB has gotten many respected scientists and consultants involved in their studies.

The following criticisms of the SR 97 performance assessment should not in any way be viewed as detracting from SKB's real accomplishments over the years.

My training has been primarily in the areas of ground-water flow and ground-water geochemistry and those are the areas in which I can profess some expertise. I have little expertise in other areas, such as canister issues, and in those areas I have taken the perspective of a lay person in reading through the SR 97 performance assessment.

I have grouped my comments on the main report into several general issues and subsequently by pagination within those issues. The issues discussed appear in the following order, which is not necessarily representative of their degree of importance in the SR 97 performance assessment: 1) stability of the bentonite barrier, 2) flow-modeling assumptions, 3) climate change and its effects, 4) independence of SKB's performance assessment, 5) miscellaneous issues and 6) coupling of scenarios. Additionally, a section on simple scientific and editorial mistakes has been added in an appendix. Although not as important as the other topics discussed in this review, editorial and scientific mistakes do affect the way SKB presents its work to the general community and consequently influence the assessment of SKB by both the scientific and lay communities.

1) Bentonite barrier issues

The main report never discusses (e.g. see p. 169) why the canister is not expected to sink through the bentonite. Presumably the canister will be denser than the surrounding bentonite and consequently it should sink, if the medium in which it is placed undergoes plastic deformation, i.e. a property which SKB expects the clay to have given its expected "self-healing" properties. Although this is never said explicitly in the report, it would be my guess that SKB doesn't expect the canister to sink significantly because of the high swelling pressure of the Na-bentonite, which may increase the viscosity of the clay to an extent sufficient to prevent sinking of canister through the bentonite. A question which is not well discussed in the main report is**: How would changing the initially pure Na-bentonite to an almost pure Ca-bentonite affect the properties of the clay?** What would be the effect of an unevenly distributed change in the properties of the bentonite as it comes into contact with $CaCl_2$-rich water at specific fracture/joint openings in the canister vault? Could this result in a tilting of the canister? The contacting water may well be a shield brine with a very high Ca/Na ratio and consequently would be expected to strongly affect the properties of the clay as well as its swelling properties. The heat capacity of the bentonite barrier would also be affected and therefore this could also have an impact on the maximum temperature around the canister. SKB should clarify all these points.

The report mentions the **possible illitization of the bentonite** buffer (p. 50). It is not at all clear that SKB considered the effect of the possible intrusion of seawater into the repository. Sea water has a considerable potassium concentration, many times higher than that of the ground waters presently observed at the 3 sites investigated.

On this same topic, on p. 201, table 8-11, SKB gives estimates for the illitization of montmorillonite based on the supply of potassium. The problem with their assessment is that it doesn't take into account the possibility of Baltic water intrusion (which presently has about 100 mg/L potassium near Aberg) or the possible intrusion of seawater (which would have about 400 mg/L potassium). If the greater possible supply of potassium is taken into account, this would mean that about 30% of the montmorillonite could be converted after 1 million years (assuming present Baltic water concentrations of potassium remain next to the near field through out that time) or even complete conversion of the montmorillonite to illite after 800000 years, assuming potassium concentrations near seawater levels. Therefore, SKB may wish to revisit this issue and assess more carefully the possibility of prolonged seawater intrusion near repository depth at

Aberg and Beberg, as well as examine more carefully the possible rate of illitization and its dependence on various environmental factors.

On p 279, **the issue of colloid transport** is raised and discarded because the "high mineralization" of the ground waters does not result in significant colloid suspension. In this regard the potential intrusion of glacial meltwaters (predicted in the climate scenario) may be problematic because these waters would be expected to be very dilute, and could therefore cause significant colloid suspension. As a result, colloidal radionuclide transport and possibly bentonite buffer erosion are two issues that should be investigated further as part of the climate scenario. These issues do not seem to be adequately addressed in the context of the climate scenario.

2) Flow-modeling issues

The SR 97 report mentions at several points throughout the report (e.g. p. 157, p. 159) the large contrast between the hydraulic conductivity of fracture zones and the hydraulic conductivity of the rock mass. These statements suggest that SKB essentially considers only two flow domains of interest at the 3 different sites. This simplistic view permeates the report. In actual fact, there is a continuum of hydraulic conductors throughout the rock, ranging from "primary" fracture zones to less extensive and possibly less conductive individual fractures. **SKB's view seems to be that so-called "second-order" and "third-order" fractures can be neglected as conductors.** Actually, although such fractures do not, on an individual basis, transport as much water as one of the more extensive fracture zones, their much greater number could make them important water conductors, which should not be neglected in SKB's analysis. The hydraulic importance of second and third order fractures should be properly evaluated by SKB, on an aggregate rather than on an individual basis.

On p. 251, the report mentions that numerical flow modeling calculations were not done with a code capable of simulating density dependent flow. Instead environmental heads were used. It seems to me that this is a significant gap in SKB's modeling effort.

On p. 275, the report mentions that the **maximum matrix penetration depth used for the radionuclide transport model is not important** because the actual penetration depth of the raionuclides is much smaller. **This statement may apply to the transport of strongly sorbing radionuclides, but does not apply to that of non-sorbing or weakly sorbing radionuclides.**

On p. 278, the statement is made that the model-calculated travel times at Aberg (for transport from the repository to the surface) are compatible with observations of very old waters at repository depth. **The fact that the waters are old at repository depth actually has very little bearing on the transit time from the repository to the surface.** At best, the ages only reflect the possible extended travel time between the surficial recharge area and the repository. It does not have anything to do with how long it will take the repository waters to **discharge** to the surface.

On p. 310, the report summarizes the "reasonable" and "pessimistic" flow-wetted surface areas (per volume of water), a_w, used for the transport calculations and the resulting advective travel times. Given the flow-wetted surface areas used in the transport calculations and given the average fracture spacing at each site (equal to twice the maximum penetration depth used in the transport calculations), we can calculate the effective porosities that should be applicable to the transport model at each site. The wetted surface area can be related to the average fracture aperture, f_a, by the relation $a_w = 2/ f_a$. The effective porosity, n, can then be calculated knowing the average fracture spacing, s, by $n = f_a/s$, or $n = 2/(a_w s)$. The results are given in the table below and compared to the porosities assumed by SKB in their transport models of the 3 sites.

Site	a_w in m^{-1}	f_a in m	s in m	n calculated	n assumed
Aberg reasonable	10^4	$2x10^{-4}$	4	$5x10^{-5}$	10^{-3} to 10^{-4} at all sites
Aberg pessimistic	10^3	$2x10^{-3}$	4	$5x10^{-4}$	
Beberg reasonable	10^4	$2x10^{-4}$	4	$5x10^{-5}$	
Beberg pessimistic	10^3	$2x10^{-3}$	4	$5x10^{-4}$	
Ceberg reasonable	10^4	$2x10^{-4}$	40	$5x10^{-6}$	
Ceberg pessimistic	10^3	$2x10^{-3}$	40	$5x10^{-5}$	

The internally consistent porosities that I calculate from the wetted surface areas and fracture spacings used in the SR 97 report are 1 and 2 orders of magnitude lower than the porosities actually used in the SR 97 transport modeling effort. This suggests that 1) the resulting model-calculated advective travel times may either be too long by 1 or 2 orders of

magnitude or 2) the wetted surface area and/or fracture spacing (i.e. max. penetration depths) values used for the transport calculations may be too high by 1 or 2 orders of magnitude. The relation that I used to relate the wetted surface area to the average fracture aperture likely provides a minimum estimate of the fracture aperture, since fracture surface roughness is not taken into account, but I don't believe that this would be responsible for an order of magnitude difference.

On p. 314, I disagree with the statement that is made that "only pessimistic values are used for delay time…and maximum penetration depth in the rock matrix". **The maximum penetration depths used are highly optimistic values.**

3) Climate Change and the Oxygenated Glacial Meltwater Issue

Bottom of p. 193, top of p. 194: SKB claims, citing the Gascoyne (1999) and the Guimera et al (1999) reports, that "there are no indications that iron(II) minerals have been oxidized by oxygenated groundwater anywhere at repository depth". The major problems with this statement are**: 1) the cited reports did not actually look for, or comment on, any reported field evidence of iron(II) mineral oxidation at depth, and 2) the statement simply ignores the field evidence presented by Glynn et al. (1997), Glynn et al. (1999) and Glynn and Voss (1999)**. At the very least, SKB should mention that their opinion, with respect to the possible intrusion of oxygenated meltwaters, is not believed by all scientists. They should definitely cite all the pertinent reports on both sides of the issue. Not to do so is unprofessional and may lead external researchers and eventually the greater public to suspect that SKB has not been forthright in its performance assessment, and that SKB is avoiding mention of issues and facts that may be unfavorable to their selected repository design.

On p. 244-248, there is a nice discussion regarding radionuclide solubilities in the context of the canister defect scenario. Unfortunately, this discussion is not repeated in the climate evolution scenario, with due consideration to the possible impact of the contact between the fuel and oxygenated waters.

On p. 317, the statement is made that "the results should be viewed in the light of the fact that extensive glaciations are to be expected in Sweden within a period of a hundred thousand years, which is the subject of the climate scenario in Chapter 10. A glaciation leads to erosion of virtually the entire soil layer. Aberg can be expected to be under the sea for a large part of the

next hundred thousand years." These statements/opinions have no place in this chapter. They should be left for Chapter 10, i.e. for the discussion of the climate scenario. **Scenarios should be discussed entirely within their own limits. If discussion of the interaction between various scenarios is needed (which is actually a good idea), these interactions should then be fully discussed and afforded an entire section of their own in the performance assessment report.**

On p. 356, the report states that glacial meltwater is, like meteoric water, rich in oxygen. This statement appears to be a subtle attempt to disguise the fact that **glacial meltwater is actually likely to be much richer (by 3 to 5 times at least) in dissolved oxygen than normal atmosphere-equilibrated water** (Glynn et al., 1997; Glynn and Voss, 1999; Glynn et al., 1999).

The climate scenario chosen for SR 97 differs markedly from the one chosen by SKI for the SITE-94 project (King-Clayton and others, 1995) from a common starting point based on SKB work. One of the main differences is the smaller extent of the ice-sheet expected during the first two glacial periods, particularly during the second one. Conveniently for SKB's performance assessment, their SR 97 climate scenario has only the ice marginal zone reaching Aberg during that glacial cycle (between 60000 and 70000 years). This is in marked contrast to the SITE-94 climate scenario where the ice sheet was assumed to reach a height of 2 to 3 km over Aberg during the second glacial cycle.

On p. 363, the report makes the statement that the oxygen dissolved in glacial meltwaters will be consumed mainly by reactions with the minerals in the geosphere. While we agree that the geosphere minerals will react with dissolved oxygen, the statement gratuitously implies that **all** the dissolved oxygen will be reacted away, i.e. consumed. This is a misleading statement that is not backed up by any substantial field evidence (Glynn et al., 1999, Glynn and Voss, 1999).

On p. 370, in the discussion of the effect of glaciation on Aberg groundwater flows, it would have been much more useful if the report had given order of magnitude estimates for the expected increase in ground water flow, instead of using purely qualitative statements.

The transport of oxygen-rich meltwater is discussed briefly on p. 379 of the report. The discussion does not mention at all the fact that some scientists (myself in particular) consider that oxygenated meltwaters could indeed penetrate to repository depths and that oxygenated conditions at that depth could remain so for significant periods of time (thousands of years). SKB discounts this possibility, primarily on the basis of 2 reports, one by Guimera et al. (1999)

and another one by Gascoyne (1999). **Given that both reports have significant flaws and that the Guimera et al. (1999) report actually states that the geochemical model used in its calculations was "optimistic", i.e. not at all "conservative", SKB is being disingenuous by ignoring other scientific opinions. The Guimera et al. report actually states, despite its "optimistic" calculations, that fast flowing fractures could indeed bring oxygenated water to repository levels.**

Furthermore the discussion misleadingly implies that the results of the Guimera et al. (1999) report were checked by Gascoyne (1999). In fact, the Gascoyne report did not check the method or calculation results of the Guimera et al. report. The discussion misleadingly states that there are no geological indications that oxidizing water has occurred at repository depth. It also fails to mention that there is no geological evidence proving that reducing conditions have always been maintained at depth over the last 100000 years. **In fact, on balance the geological evidence suggests, albeit does not conclusively prove, that oxidizing conditions probably did occur at repository depth over the past 100000 years (Glynn et al., 1997, 1999; Glynn and Voss, 1999). Despite the earlier statement about lack of geological evidence, the SR 97 report actually mentions possible evidence from Finland (without citing references!) that does suggest that oxidizing conditions possibly penetrated to significant depths during the last glaciation.**

Furthermore, the discussion in the SR 97 report of the conclusions and results of the flow modeling work done by Svensson (1999) supports the earlier modeling results found by Provost et al. (1998) and incorporated in Glynn and Voss (1999). The discussion in the SR 97 report contradicts many of the erroneous statements made by Gascoyne (1999), who primarily discussed the flow and transport modeling work of Provost et al. (1998).

On p. 381 and 382, the report provides some water analyses that may be representative of glacial meltwaters after reactions in a fractured rock environment. The report does not provide references for these analyses, but more importantly misleadingly claims that the two waters (from Grimsel and Taavinunnanen) differ substantially in their chemistry from a glacial meltwater analysis that is also provided. First of all, the report fails to mention that the water at the base of an ice sheet might differ substantially from the water collected from the outlet of a mountain glacier. Secondly, although the Grimsel and Taavinunnanen waters indeed contain more solutes than the glacial meltwater, they nevertheless are still exceedingly dilute compared

to most normal ground waters, and more importantly there is absolutely no evidence that they are reducing waters. There are no Fe or Mn or sulfide concentrations given, so the concentrations of these indicators of reducing conditions must not be very important, otherwise they would have been provided. The only redox sensitive compound for which concentrations are provided is sulfate. This suggests that the Grimsel and Taavinunnanen waters are actually oxidizing waters and may even contain dissolved oxygen, although no measurements are given. Therefore, by themselves, the water analyses provided by SKB contradict their own conclusions regarding the potential for deep penetration of oxygenated water.

On p. 441, the report mentions that "there is a very great potential for oxygen consumption in the minerals in the geosphere". This statement, while strictly true, is misleading because it ignores the fact that 1) access of the waters to all this reductive mineral mass may be very limited and 2) the kinetics of reaction of these minerals are generally extremely slow. In other words, there are very good odds that the "very great potential for oxygen consumption" will never be realized.

Finally, on p. 442 the report mentions that oxygenated water is not expected to infiltrate to repository depth other than during "very limited" periods. It would be useful if SKB could quantify the "very limited periods" and also of course provide the appropriate range of uncertainty for their analysis. This would better show SKB's confidence in their statement.

4) Independence of SKB's Performance Assessment Efforts

On p. 440, the report makes the blanket comment "A comparison with safety assessments in other countries shows that the set of scenarios that is analyzed in SR 97 agrees very well with other assessments". The question in this reader's mind is: to what extent were these assessments independent? This is a important question which should be addressed by SKB. In my experience, I get the impression that international "experts" on nuclear waste disposal issues often work for different countries and/or agencies on performance assessments and that the same sources of knowledge are "shared" between assessment efforts. Therefore, the true independence of these efforts is questionable.

5) Miscellaneous issues

p. 140 and 141. It would be nice if the report mentioned why the chemotoxicity of Pu and U, which differs from their radiotoxicity, can be considered insignificant in the safety analysis. Nothing is said about this subject in SR 97.

Although on p. 184, SKB lists processes that are influenced by the composition of pore waters, there is no effort made to list the rate estimates for such processes. The rates of several of these processes are crucial in understanding to extent to which the near-field barriers will be able to maintain their function over the desired lifetime of the repository.

On p. 206, when discussing the potential for sulfide corrosion of the copper canisters, the report mentions that "pyrite is evenly distributed throughout the buffer and that there is no reason to expect local attacks". I don't see why local corrosion could not be expected particularly in a environment (the bentonite) where the migration of ions will proceed only by diffusion rather than by advection. Even if the pyrite appears "evenly" distributed, there is bound to be significant changes in the composition of the porewaters (in sulfide activity and in pH and EH conditions) next to the canister, on a cm scale or smaller. Such changes could cause enhanced corrosion of the canister in some spots.

On p. 223, the report mentions that the requirement is that the k_{eff} value not exceed 0.95. Given that criticality will occur at a value of 1, from a layman's perspective the target k_{eff} value of 0.95 seems rather high, i.e. it does not appear to leave much of a safety factor. The discussion of criticality, the precautions taken to avoid it and the consequences of its possible occurrence, appears a bit meager to me.

On p. 377, the report mentions that the total pressure on the canister during a glaciation is expected to be about 39 MPa and that the canister inserts have been calculated to withstand an external evenly distributed pressure of 80 MPa or 110 MPa, depending on the actual design used. This analysis, however, probably does not take into account the possible weakening of the canister insert because of corrosion or other effects. Consequently, the safety margin regarding the design of the canister insert would appear to be rather small.

On p. 411, the discussion of canister failures and canister damages caused by earthquakes is rather confusing, possibly because a "damaged" canister may not necessarily represent a canister "failure".

6) Lack of Coupling between Scenarios

In general, one of the problems with the climate scenario, is that there is little coupling between the chemical and hydraulic evolution of the near-field and far-field systems and their mechanical evolution (particularly for the near-field).

On p. 414, the SR 97 report mentions that in the earthquake scenario analysis no credit has been taken for the fact that it **will** be possible to reject "unsuitable" canister positions. It is quite interesting to read this statement for this scenario, and to contrast it with the exact opposite statement which is made in the Guimera et al. (1999) report, with regards to the climate scenario. In that report, credit is claimed for the fact that it will be possible to reject "unsuitable" canister positions. All in all, SKB's approach and methodology seems a bit inconsistent and apparently depends on the seriousness of the studied scenario.

As a general comment, I think that the earthquake and climate scenarios should have been explicitely linked together in a separate scenario, given the strong coupling between deglaciation and earthquake frequency.

On p. 442, the report states that "The overall conclusion of the climate scenario is that the climatic evolution does not lead to failure of intact canisters". Again, this is misleading because the climate scenario does not examine the impact of glaciation and deglaciation on corroded or defective canisters. (The corrosion of the canisters does not necessarily have to occur from the presence of oxidizing waters, it could also occur from localized sulfide corrosion. Also, the report never examines the impact of earthquakes as part of the climate scenario, on these corroded canisters).

Conclusions

This review has identified many technical problems in the SR 97 performance assessment. The general impression of this reviewer is that SKB has been disingenuous in its performance assessment effort. It has not cited important differences of opinion with its own views. Furthermore, there are many inconsistencies in the SR 97 report that all together leave the impression that there are many more uncertainties in the SR 97 performance assessment than SKB would perhaps care to admit. Additionally, despite SKB's statements to the contrary, many of the analyses conducted for the SR 97 performance assessment can be clearly shown not to have been based on "conservative" assumptions. Finally, SKB has made little effort to consider

possible coupling effects between their different scenarios in SR 97. This is a serious flaw in the SR 97 performance assessment.

The comments in this review should not be taken to imply that the KBS-3 nuclear waste disposal method will not be able to meet the safety and radiation protection requirements which SKI and SSI have specified in recent years (p. 456). Instead, my conclusion is simply that the SR 97 performance assessment of the KBS-3 method would have been more believable had it been based on a forthright and comprehensive discussion of facts, uncertainties and opinions, and on a more conservative choice of assumptions. As it stands, the SR 97 performance assessment is not very credible.

Appendix

Simple Editorial/Scientific Mistakes:

As a general policy, SKB should try to ensure that their public documents receive adequate technical and editorial review to ensure that mistakes such as those mentioned below do not see the light of day in future reports. Although not particularly important from a scientific point of view, the mistakes reflect on SKB's professionalism and will impact the impression that their published documents will give to lay readers and journalists regarding SKB's competence.

SKB should also have a formal mechanism set up by which they could officially (in print and with wide public distribution) retract, or correct, the results of any prior reports that they might have published that they might believe were in substantial error. Any retraction or correction should of course be fully explained and justified. I know of at least one, and possibly two, reports that SKB managers have professed, through verbal communication, to be in error. Leaving this issue aside, the following illustrates some of the scientific and editorial mistakes made by SKB in their SR 97 main reports.

On p. 117, SKB mentions that asphalt occurs as a fracture-filling mineral. This must be a mistake. I know that the deep hole in the Siljan ring was drilled in the exploration for petroleum in the Scandinavian shield, but this observation of natural asphalt is really news to me.

On p. 189 and then again on p. 191, the report mentions that the Aberg and Beberg water compositions are in thermodynamic equilibrium with hematite and goethite. This is for all practical purposes impossible. The water is likely to be at equilibrium either with respect to

hematite, or with respect to goethite, but not with respect to both. It is surprising that SKB should not be able to catch significant mistakes such as this one. Mistakes like this probably do not significantly affect the performance assessment, but they nevertheless demonstrate a lack of competent technical and editorial review. If simple matters like this are wrong, how can SKB maintain credibility on more serious matters?

On p. 208, the report mentions that "Models that deal with groundwater composition and evolution in different ways are not used directly for predictions in the safety assessment". This statement is plainly wrong. To cite one example, SKB has used some (but not all) of the model results of Guimera et al. (1999) to predict that oxygenated water will not get to repository depth. On that basis, SKB decided to disregard the possibility of oxygenated meltwater intrusion.

On p. 212, SKB makes the comment that "the buffer material is taken from a natural environment where conditions have for millions of years resembled conditions at repository depth in Swedish bedrock". I would argue that both the environmental conditions responsible for the formation of the bentonite and the present environmental conditions where the bentonite is found are actually quite different from Swedish bedrock conditions.

On p. 330, the report makes the comment "The effects of uncertainties surrounding the properties of the buffer as regards radionuclide transport are small. Provided that the buffer's long-term evolution is as in the base scenario, our understanding of the buffer's role in radionuclide transport is good." This statement is essentially similar to saying that provided that there are no uncertainties regarding our understanding of the buffer's long term evolution, there are no significant uncertainties regarding the properties of the buffer. This is an example of circular reasoning. Actually, there may be significant uncertainties regarding the long-term evolution of the buffer and of its properties, and to this reader it simply sounds like SKB is trying to disguise this fact.

On p. 415, first line, the report reads "The frequency assumptions in the risk analysis are thus not pessimistic if a glaciation with subsequent deglaciation should occur within the next hundred thousand years." In other words, the frequency assumptions are optimistic! It is interesting to see the linguistic convulsions to which SKB will lend itself to avoid admitting possible design vulnerability.

On p. 365, two paragraphs one for Aberg and one for Beberg are repeated by mistake.

References

Guimera, J., Duro, L., Jordana, S., and Bruno, J., 1999, Effects of ice melting and redox front migration in fractured rocks of low permeability, SKB Technical Report TR-99-19, 86 p.

Gascoyne, M., 1999, Long-term maintenance of reducing conditions in a spent fuel repository: A re-examination of critical factors, SKB Report R-99-41, 56 p.

Glynn, P.D., Voss, C. and Provost, A., 1997, Glaciation and ground-water geochemistry in the Fennoscandian Shield: Deep oxygenated ground water of glacial origin, *in* Glaciation and Hydrogeology: Workshop on the impact of climate change and glaciations on rock stresses, groundwater flow and hydrochemistry - Past, present and future, King-Clayton, L.M., Chapman, N.A., Ericsson, L.O., and Kautsky, F. eds., Proceedings of a Workshop, Stockholm, Sweden, April 17-19 1996, SKI report 97:13.

Glynn, P.D., and Voss, C.I., 1999, Geochemical Characterization of Simpevarp Ground Waters near the Äspö Hard Rock Laboratory, Swedish Nuclear Power Inspectorate (SKI), SKI report 96:29, 210 p.

Glynn, P.D., Voss, C.I., and Provost, A.M., 1999, Deep penetration of oxygenated meltwaters from warm based ice sheets into the Fennoscandian Shield, in Use of Hydrological Information in testing groundwater flow models: Technical Summary and Proceedings of a Workshop organized by the NEA Coordinating Group on Site Evaluation and Design of Experiments for Radioactive Waste Disposal (SEDE) and by the Swedish Nuclear Fuel and Waste Management Company (SKB), Borgholm, Sweden, September 1-3, 1997, p. 201 - 241.

King-Clayton, L.M., Chapman, N.A., Kautsky, F., Svensson, N.-O., de Marsily, G., and Ledoux, E., 1995, The central scenario for SITE-94: A climate change scenario, SKI report 95:42, 134 p.

Provost, A., Voss, C., and Neuzil, C., 1998, Glaciation and regional ground-water flow in the Fennoscandian shield, Swedish Nuclear Power Inspectorate, SKI Report 96:11.

Svensson U, 1999, Subglacial groundwater flow at Äspö as governed by basal melting and ice tunnels. SKB Report R-99-38.

The author

Dr. Pierre D. Glynn is a senior scientist for the U.S. Geological Survey, Water Resources Division, National Research Program in Reston, Virginia (1987 to present). He also serves as an associate editor for the journal Ground Water. Dr. Glynn's professsional training is in the areas of low-temperature geochemistry, isotopic geochemistry and ground-water flow and transport processes. He has a B.A. from Columbia University (1980), M.Sc. from University of Quebec in Montreal (1982), and Ph.D. from Waterloo University in Canada (1986). Dr. Glynn's present research interests concern: 1) the geochemical evolution of ground-water systems, 2) the reactive transport of contaminants in ground water, 3) radionuclide solubility and sorption modeling, 4) the thermodynamics of solid-solution aqueous-solution processes, and 5) ground-water dating with geochemical and isotopic techniques. In addition to conducting research, Dr. Glynn often teaches courses on ground-water geochemistry and transport processes. Dr. Glynn has been involved in conducting research on nuclear waste disposal issues since 1992, primarily for SKI, but also for the U.S. Department of Energy.

Evaluation of Heat Propagation from a KBS–3 Type Deep Repository for Aberg, Beberg and Ceberg in SKB's SR 97

Patrick Goblet[1]
Ghislain de Marsily[2]

[1]Centre d'Informatique Géologique, Ecole Nationale Supérieure
des Mines de Paris, 35 Rue Saint-Honoré
77305 F – FONTAINEBLEAU, France

[2]Laboratoire de Géologie Appliquée, Université Pierre & Marie Curie,
4 Place Jussieu
75252 F – PARIS, France

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Contents

1. Introduction

In December 1999 the Swedish Nuclear Fuel and Waste Management Co delivered to the Swedish Nuclear Power Inspectorate the performance assessment SR 97, a PA of post-closure safety for a deep repository for spent nuclear fuel.
In a PA, one important issue to consider is heat propagation from the fuel in a repository and its influence on technical and natural barriers. The thermal output of spent fuel can influence the mechanical and geochemical evolution on the near-field and also have an impact on the response of the far-field to climate change.
The objective of this study is to complement a bibliographic study performed by ARMINES for SKI on the characterization and modeling of heat transfer mechanisms around a HLW repository. The study is concerned with the analysis of SR 97 documents describing the heat propagation modelling work performed on the national sites Aberg, Beberg and Ceberg.
The following documents were reviewed:

Ageskog, L., Jansson, P.: *Heat propagation in and around the deep repository – Thermal calculations applied to three hypothetical sites: Aberg, Beberg and Ceberg*. SKB TR 99-02, 1999.

Deep repository for spent nuclear fuel. SR 97 – Post-closure safety. SKB TR 99-06, 1999.

SR 97 – Processes in the repository evolution. SKB TR 99-07 1999.

SR 97 – Waste, repository design and sites. SKB TR 99-08 1999.

SR 97 – Data and data uncertainties – Compilation of data and data uncertainties for radionuclide transport calculations. SKB TR 99-09 1999.

Additional references used are listed at the end of the report.

2. Description of the medium

The geological medium is modelled as an Equivalent Continuous Medium. This approach is justified for heat transfer calculations in very low permeability rocks, since it has been shown that conduction is the dominant process. Other types of models (discrete fracture or double porosity models) might be appropriate to model the consequences of heat load in terms of rock mechanics or chemistry, but this is beyond the scope of the present work.

3. Mechanisms

The mechanisms which are likely to occur are analysed in [9] and [10]. We shall briefly review them and see whether the modelling work done in [2] is consistent with this phenomenology. The material for this discussion is from [9], section 8.6.

The primary heat transfer mechanism is located inside the canister: heat is transferred by conduction inside the fuel, by conduction and radiation between the fuel and the cast iron insert, and finally by conduction and radiation between the insert and the copper canister. The detailed evolution of this system is complex to predict, but is of no relevance in the study discussed here, because in a very short time period, the heat transfer from the container and the surrounding medium is actually driven by the heat output function, which is well known, and by the properties of the surrounding medium.

In the modelling work, the canister is therefore modelled as a homogeneous unit, with average thermal properties.

Heat transfer in the buffer material is by conduction when the buffer is saturated. During the initial phase where the bentonite is not fully saturated, and is furthermore subject to a moisture redistribution mechanism due to the heat, an additional component to heat transfer is convective vapour transfer. On the other hand, the heat transfer parameters of the bentonite depend on the water content.

In the modelling, vapour flow has been neglected, which is conservative. The uneven spatial distribution of the thermal conductivity has been modelled in a simplified way, by a concentric zoning of this parameter which does not vary with time.

Finally, heat transfer in the geosphere is mainly by conduction. The convective transfer by flowing water is neglected. This assumption has been shown to be appropriate for realistic situations, see e.g. [3].

It is stated in [9] (p. 145) that the weak point of thermal modelling is generally not in the representation of a particular component, but in the heat transfer between different components. This particular aspect is addressed in [2] for the transition between the canister and the bentonite (effect of an air gap).

4. Parameters

The heat transfer mechanisms are controlled by different parameters depending on the scale considered: on a local scale, the heat conductivity and heat capacity of bentonite play the leading role. The heat conductivity depends on the moisture distribution in the buffer. Bounding values have been used which cover situations from a very dry bentonite to an almost saturated

one. This parameter is only important on a short time scale, to assess the maximum temperature at the canister boundary. Uncertainties regarding the long term evolution of thermal conductivity should therefore not affect the results.
The heat transfer properties of gaps between the canister and the bentonite depend of the emissivity of the media (copper and bentonite), which is not precisely known in repository conditions. Conservative values have been used in the calculations.
Finally, global heat transfer depends essentially on the heat conductivity of the rock mass. This parameter varies over a rather restricted range depending on the rock type. The typical values used in the study come from numerous in situ measurements. They can be considered as representative of the various media considered. Furthermore, they cover a sufficient range to permit an analysis of the influence of this particular parameter.
One may finally note that the values retained for the thermal parameters are consistent with values generally used in the literature (see [4]).

5. Discussion of approaches and results

The modelling approach includes three steps corresponding to different, embedded scales:

- Local model: the immediate vicinity of a canister is modelled. At this scale, the effect of gaps between the container and the bentonite is studied.
- Intermediate model: a "unit cell" surrounding a single canister is modelled, to investigate the relationship between initial thermal load and borehole spacing
- Global model: the progressive emplacement of canister is modelled, and the long term temperature evolution is computed.

In this section we analyse the representation of the various components of the modelled system, from the local to the global scale.

5.1. Source-term

The canister is represented as a cylindrical, homogeneous structure. Although Figure 4-2 in ref. [2] suggests the possibility to distinguish inner part and casing, the material properties assigned to each region are in fact identical. This simplified approach is justified in view of the calculation scale. Only one reference discussed in [4] mentions a more detailed approach: in [8], the canister is represented by a series of concentric, cylindrical media with different thermal properties. This approach however is only justified by the possibility to consider different canister designs.
The canister initial heat output is in the high range compared to most previous Swedish calculations. This reflects the present trend to make maximum use of the canister capacity due to its high cost.

5.2. Buffer material

The modification of water content with time is not taken into account in the modelling. This seems reasonable, since the detailed modelling of the coupled heat and flow transfer is still in a research stage. However, the modification of the buffer properties due to water redistribution is represented in a simplified way: three concentric zones are considered, with an increasing water content from the container to the host rock. This approach is consistent with experimental observations done during heating experiments, e.g. the Japanese Big Ben experiment ([6]) or the Kamaishi Mine experiment ([7]). One should note however that these experiments lead to saturation values lower than the values considered in the present study. In view of this, it appears justified to have chosen thermal conductivity values in the low range for the inner part of the buffer.

5.3. Influence of air gaps between container and bentonite

Due to the difficulty of ensuring a perfect contact between container and buffer blocks, and between buffer and surrounding blocks, air gaps are expected to remain at the time of closure of a borehole. These gaps should normally be filled with water, and closed by the swelling of the bentonite. However, the heat produced by the waste container may hinder for an unknown period of time a sufficient moisture to seal the gaps. This possibility has been considered in previous studies ([1], [5], [8]). The phenomenology considered in the present study is identical to that of the quoted references: heat transfer is by conduction and radiation, convection is neglected. Radiation is represented here by an increase of the apparent thermal conductivity of the medium, as in [8]. The apparent conductivity due to radiation is based on realistic values of the emissivity of materials (copper and bentonite). Finally, a local heat transfer model permits to dimension the properties of the gaps in such a way as to obtain the maximum temperature jump while retaining realistic parameter values. Although the details of this model are not given, the order of magnitude of the results can be checked with a simple steady state calculus: with a heat flux of $1625 / (2\pi \times 0{,}5 \times 4{,}8) = 108$ W/m^2, and an equivalent thermal conductivity of 0,08 W/m °C (corresponding to an air gap of 10 mm and to a “normal” emissivity of copper), the temperature jump across a 10 mm gap is 13,5 °C, consistent with the results of figure 4-1 in [2].

(**Note**: in [10], p. 99, a temperature jump of 30°C is quoted across an air gap between container and buffer. It would be useful to check where the difference with the present results comes from).

In view of these results, it appears justified, either to model air gaps by a modification of the thermal properties of the medium if the spatial discretization is sufficiently fine, or to include the temperature jump in the target temperature at canister surface, as is proposed in this study, for a large scale calculation.

5.4. Borehole spacing

Borehole spacing calculations are based on a local model: a "unit cell" bounded by vertical symmetry planes and including one quarter of a container is modelled. A similar approach is followed for instance in [5], [11], [8], [12], [13]. This unit model is appropriate to describe an infinite number of galleries of infinite length, and is therefore conservative from the viewpoint of the temperature increase.
Upper and lower boundary conditions are not described, but probably these limits are sufficiently far to have a negligible effect.
One may note that the unit cell concept gives a common framework for the three investigated sites: given a gallery spacing and a borehole spacing, the geometry of the modelled domain is the same for all sites. The only site specific data are the thermal parameters (conductivity and specific heat) and the initial temperature of the medium (the natural thermal gradient is not taken into account). Due to this similarity, the differences between the three sites reflect essentially differences regarding the above mentioned parameters. To make this point clear, let us consider the general heat conduction equation:

$$\mathrm{div}\{\Lambda_t \,\mathrm{grad}\, \theta\} = \rho C \frac{\partial \theta}{\partial t} + \varphi$$

where λ_t is the total conductivity of the medium, θ the temperature, ρC the volumetric heat capacity, t the time, and φ a thermal source term. It is apparent from this equation that if λ_t is scaled by a factor K1, and θ by a factor K2, then φ will be scaled by a factor K1×K2, and time by a factor 1/K1 (or a different factor if ρC is scaled as well). If the source term is constant, its value can therefore directly be deduced from K1 and K2. If on the other hand, the flux is not constant, then the scaling of time will destroy the similarity of behaviours, because φ is not properly scaled for time.

For instance, if we compare the results for sites Aberg and Beberg, we have K1 = 3,2/2,8 = 1,14, and K2 = (80-13,5)/(80-16) = 1,039. The ratio between admissible (constant) load for sites Aberg and Beberg should be 1,184. From the curves of figure 4-3 in [2], we have a ratio of 1,128 for a 6 m interval between boreholes, and 1,11 for a 9 m interval. Similarly, for Aberg and Ceberg, we have K1 = 1,36, and K2 = 1,078. One would expect a ratio between admissible loads of 1,47. The calculated ratio is 1,29 for 6 m interval, and 1,25 for 9 m interval. One can see that the ratio between admissible loads for two sites is closer to the theoretical ratio when the borehole spacing is smaller, because the maximum temperature is reached sooner, and the source term deviates less from the constant source hypothesis. This discussion shows that the modification of admissible load is not readily deduced from a modification of the parameters, and justifies the numerical approach taken in the study.

5.5. Long term thermal evolution

The large scale simulations allow to model the site specific geometry in a more realistic way, and to take into account the progressive emplacement of canisters. The scale of the models is much larger than in the previous calculations: the vertical boundaries are at a distance of about 1000 m of the actual repository boundaries. To achieve these simulations with tractable meshes, it has been decided to simplify the source term modelling: only galleries are represented in the mesh, in the form of lines of Finite Element nodes. The heat source is

uniformly distributed along these lines. While this approximation is perfectly justified as far as long range influence is considered, one must keep in mind that the dilution of the thermal source term in the influence domain of nodes creates a bias for short range temperatures: the temperature field is smoothed, and the actual maximum temperature is underestimated. This is clearly visible on temperature fields calculated at the beginning of deposition phase II, where maximum values of 35 to 45 °C at most are found, while the dimensioning calculations provide for a 80 °C maximum.
The average temperature fields calculated on the large scale meshes are probably valid for long term calculations (200 and 1000 years). It would be interesting to use the local unit cell model to determine when the temperature levelling is effective.
With this restriction in mind, we consider that the large scale calculations are probably appropriate to describe the interaction between galleries, and between repository levels for Aberg.

6. Numerical technique

The numerical tool used to model heat transfer represents current state of the art technique. The heat conduction equation does not pose any particular problem, and the spatial discretization seems appropriate to describe the smooth temperature fields simulated. The effect of mesh size in the immediate vicinity of the galleries has however an influence on the average temperature at an early stage of the calculations. This point should be investigated (as should, more generally, the transition from the local unit cell to the global model).

7. Influence of temperature on other processes

An important aspect of the present review was “the influence of the temperature on the mechanical, geochemical and hydrological processes in the near-field and the far-field of the repository”. A comprehensive analysis of these aspects would be well beyond the scope of this study, and would entail a much larger bibliographic review. However, we have studied the reviewed references to see whether these aspects were addressed in SR 97, and to what extent.

7.1. Influence on flow

The coupling of water saturation of the buffer to the thermal evolution is mentioned in [9], p. 162. The details of the modelling approach are not yet published.

The influence of temperature on flow in the rock mass does not seem to be addressed in SR 97.

7.2. Influence on mechanical behaviour

Thermal evolution has an effect on the mechanical behaviour of the buffer and the surrounding medium, due to the thermal expansion of the water and of the rock mass. The phenomenology is described in details in [9], from the canister scale to the rock mass scale. Simulation results are shown for the evolution of the stress state with time. These results come from a 1997 reference, and are computed with different hypotheses regarding the heat load (1000 W / canister).

7.3. Influence on chemical behaviour

The effect of temperature on the chemical evolution of the repository is mentioned in a general way in [9], p. 184. Specific mechanisms are discussed on pp. 199, 200: modification of barrier properties by precipitation-dissolution of Calcium sulphates and calcite, or of Silicon compounds. The influence of temperature on radionuclide speciation is mentioned on p. 243. These examples show that this fundamental aspect is addressed. It will remain an essential research topic in the coming years.

7.4. Influence on climatic evolution

The scenario for climatic evolution concerns a time frame in which the thermal influence of the repository will have practically vanished.

8. Conclusions

The following conclusions and remarks may be drawn from this review work:

The phenomenology of heat propagation in the complex system of a repository is generally well understood, and permits a reliable prediction of temperature evolution. Some simplifications such as the representation of incomplete saturation of the buffer are justified at the present stage of knowledge, and do not seem to impair the reliability of the results. These simplification may become unnecessary in the future as experimental work presently going on leads to a better predicting capacity of these mechanisms.

Important parameters (thermal conductivity and heat capacity) are known through a large number of measurements, and furthermore do not span a wide range. The main uncertainty

seems to lie in the near field parameters (description of the contact between container and buffer, thermal conductivity of unsaturated bentonite). Generally speaking, the weak point of thermal modelling is generally not in the representation of a particular component, but in the heat transfer between different components. Although no systematic sensitivity analysis was performed in this study, the various situations modelled do give an idea on the effect of varying parameters such as thermal conductivity, heat capacity, initial heat output,…

The modelling work presented in [2] is consistent with the phenomenology described. A powerful computing capacity allows a detailed description of mechanisms at two different scales. However, the transition from one scale (unit cell) to the other (global scale) would deserve a more rigorous analysis.

From a reviewer's viewpoint, the description of calculation cases is generally not sufficiently detailed to judge precisely the results, or to try and duplicate them, should this be needed. While this situation is acceptable in a generic exercise such as SR 97, a more detailed description would be required in a real site assessment.

Apart from thermal parameters and repository location and geometry, the results would be highly sensitive to hypotheses regarding the waste production (burn-up, intermediate storage,…). These aspects are not addressed in this work, but the modelling done shows well, inversely, how these parameters may be optimised from a temperature criterion.

Consequences of the thermal evolution on hydrological, mechanical and chemical phenomena are considered, but have not yet, as far as we can tell, been updated considering the latest heat transfer simulations. Chemical aspects are by far the most complex, and will require an important work in the future.

As a general conclusion, the study shows the feasibility of calculations aimed at dimensioning the repository geometry as well as its exploitation.

9. List of references

[1] Ageskog, L., Jansson, P.: *Äspö Hard Rock Laboratory - Prototype repository - Finite element analyses of heat transfer and temperature distribution in buffer and rock - general part & case No 1* . HRL-98-20, 1998.

[2] Ageskog, L., Jansson, P.: *Heat propagation in and around the deep repository – Thermal calculations applied to three hypothetical sites: Aberg, Beberg and Ceberg*. SKB TR 99-02, 1999.

[3] Chan, T., Nakka, B.W., O'Connor ,P.A, Ophori, D.U., Reid, J.A.K., Scheier, N.W., Stanchell, F.W.: *Thermohydrogeological modelling of the Whiteshell Research Area*. AECL report AECL-10947, COG-93-368, 1998 .

[4] Goblet, P., de Marsily, G.: *Evaluation of the Thermal Effect in a KBS-3 Type Repository*. SKI Report 00:18, 2000.

[5] Hopkirk, R.J., Wagner, W.H.: *Thermal loading in the near field of repositories for high and intermediate level nuclear waste.* Nagra Technical report 85-54, 1986.

[6] Jing, L., Rutqvist, J., Stephansson, O., Tsang, C.F., Kautsky, F.: *DECOVALEX - Mathematical models of coupled THM Processes for Nuclear Waste Repositories; Report of Phase III*. SKI Report 95:80, 1995.

[7] Jing, L., Stephansson, O., Börgesson, L., Chijimatsu, M., Kautsky, F., Tsang, C.F.: *DECOVALEX II Project – Technical Report – Task 2C*. SKI Report 99:23, 1999.

[8] Sato, R., Sasaki, T., Ando, K., Smith, P.A., Schneider, J.W.: *Calculations of the Temperature evolution of a Repository for Spent Fuel in Crystalline and Sedimentary Rocks.* Nagra Technical report 97-02, 1997.

[9] SKB: *Deep repository for spent nuclear fuel. SR 97 – Post-closure safety.* SKB TR 99-06, 1999.

[10] SKB: *SR 97 – Processes in the repository evolution.* SKB TR 99-07 1999.

[11] Thunvik, R., Braester, C.: *Heat propagation from a radioactive waste repository. SKB 91 reference canister*. SKB TR 91-61, 1991.

[12] Tsui, K.K., Tsai, A.: *Three-dimensional thermal and thermomechanical analyses for the near-field of a disposal vault with the borehole emplacement option*. Ontario Hydro report N-03788-940014 (UFMED), June 1994.

[13] Tsui,K.K., A.Tsai: three-dimensional thermal and thermomechanical analyses for the near-field of a disposal vault with an in-room emplacement option. Ontario Hydro report N-03788-940015 (UFMED), June 1994.

The authors

The Centre d'Informatique Géologique is one of the research centers of the Ecole Nationale Supérieure des Mines de Paris. Its activities are related to underground fluid and mass transport, and more generally to the water cycle. Underground storage of radioactive waste has been a major topic of research for more than 20 years: model development and application, characterisation of fractured rock, long-term behaviour of sedimentary structures, natural analogues etc.

Patrick Goblet is the main author of the METIS code (groundwater flow in saturated and unsaturated media, heat and mass transport in 2 and 3D), and has been involved in verification and validation projects (INTRACOIN, HYDROCOIN, INTRAVAL). He has for many years contributed to the development of the MELODIE code (Safety assessment code of the French Institute for Protection and Nuclear Safety). He has a long experience of code application in various fields, including safety assessment of deep HLW as well as shallow LLW repositories.

Ghislain de Marsily, formerly Director of the Centre d'Informatique Géologique, is now Professor of Applied Geology at the University Paris VI, and Head of a Joint Research Unit of the French National Centre for Scientific Research (CNRS) which includes both the University of Paris VI, Department of applied Geology, and the Ecole Nationale Supérieure des Mines de Paris, Centre d'Informatique Géologique. He is a member of the French Commission for the Evaluation of Research in Nuclear Waste Disposal (CNE). He has been involved in nuclear waste disposal research for more than 25 years, in France, and in several European projects and in the US.

Review of
Spent Fuel Related Issues
in SKB's SR 97

Bernd Grambow
Ecole des Mines de Nantes, SUBATECH-Laboratory
4 rue Alfred Kastler, F-44307 Nantes, France

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Preface

In preparation for coming site investigations, SKB has carried out an assessment of the post closure safety for repositories with spent nuclear fuel in deep granite formations. The results of the project are documented as a series of reports under the title “SR 97” (SKB 1999a, 1999b, 1999c, 1999d). The present review addresses spent fuel related issues in these reports in relation to the overall objectives of SR 97. Other issues (methods, scenario, canister corrosion, etc.) are addressed as far as spent fuel behavior is concerned.

The long term safety of geological disposal of spent fuel is assessed in SR 97, as in any other safety assessment, based on different types of models derived from experimental or field observations, considering diverse theories, assumptions and hypotheses. The present review attempts to evaluate whether the selected radionuclide release models for spent fuel are sufficiently well founded on experimental observations and whether the underlying theories, hypotheses and assumptions are sufficiently justified. A special concern is the methodology for concluding from short term experimental observations on the long term spent fuel performance. In certain cases alternative model and data choices are reported in the literature. It is then evaluated whether the choice taken by SKB is suitable for safety assessment. The encountered uncertainties in scenario, models, and data are in most cases not only pertinent to the approach selected by SKB but to many international projects on spent fuel performance assessment as well.

The review represents the view of the author, which is not necessarily identical to that of SKI.

Summary

The solid waste form "spent fuel" constitutes both the dominant radionuclide source as well as a first radionuclide retention barrier of a planned future high level nuclear waste isolation systems in deep granite formations. In order to evaluate the performance of spent fuel as part of the multibarrier containment system in a deep repository, the radionuclide release properties in groundwater must be predicted over very long time periods. Radionuclide release is not an inherent materials property of the fuel but depends, besides fuel specific parameters, mainly on time but as well on the geochemical and hydraulic environment of the disposal location. The study SR 97 documents the large effort of SKB to assess the long-term performance of a repository containing spent nuclear fuel. Scenario and consequence analyses are clearly described, considering major physical and chemical interactions of the various components of the multi-barrier isolation system. The approach attempts to assess both a realistic and a pessimistic evolution scenario.

The present report attempts to evaluate whether this approach is thoroughly carried through to assess the performance of spent nuclear fuel in a repository. Main issues are radionuclide inventories and inventory distribution between structural parts of the fuel assembly and the fuel matrix, potential fuel alteration prior to water access, as well as models for fuel matrix dissolution and instant release fractions.

Uncertainties in radionuclide inventories are discussed and were found for many radionuclides to be higher than assumed in SR 97. This is particularly true for Cl-36. This nuclide is a potential key biosphere dose contributor in various international safety assessments. Of particular importance are uncertainties related to the partition of radionuclides between metallic parts of the fuel assembly and the fuel matrix, since inventories of metallic parts are considered to be released instantaneously. Using C-14 as an example, it is shown that high uncertainties in release properties result from the (uncertain) choices in this partitioning.

The analyses of the fuel performance in the case of groundwater access is in SR 97 is based on the assumption that the fuel integrity and fuel oxidation states do not alter prior to water access. No account is taken for potential fuel oxidation in a defected canister during interim storage or disposal. Fuel oxidation at surface temperatures of 200-400°C during storage or disposal is expected to be fast. This process is known to strongly alter fuel integrity.

Special attention is given to processes and models which describe spent fuel dissolution and radionuclide release in the case of groundwater access to the fuel. Based on a detailed discussion of the current state of knowledge of radiation assisted fuel dissolution models it is concluded that the long term corrosion rates of the fuel matrix used by SKB with a value of 10^{-8}/year are overly optimistic. The proposed long-term corrosion rate is considered to be independent on environmental parameters such as pH, pCO_2 or of fuel specific parameters such as burnup or surface area. As discussed in this review, these assumptions are in conflict with experimental observations.

It is concluded that the SR 97 approach to the assessment for radionuclide release from spent fuel assemblies is characterized by an optimistic view which is not necessarily incorrect but which is not sustained by the base of current knowledge. A significant drawback is that the source term is not quantified based on the experimental results of a more than 20 year lasting spent fuel leaching program performed in the STUDSVIK laboratory, but rather on theoretical concepts whose quantification is poorly documented and on experimental data obtained from unirradiated UO_2.

Basic fuel characteristics

Burnup

It is assumed that 38 GWd/tU BWR fuel data are more or less representative for the large suite of fuels to be disposed off (the value of 38 MWd/tU used on Page 59 in SKB 1999a is to be considered as a typographic error). With the exception of MOX fuel, the error associated is probably small, but this is not necessarily valid for all radionuclides, particularly for activation products in the structural parts of fuel assemblies and for higher actinides. SR 97 gives only the expected average burnup of the fuel, a probability distribution function of burnup and linear power would be useful to assess uncertainties in radionuclide inventories. This is particularly important for fission products and actinides, whose formation requires capture of 2 or more neutrons (e.g. Cs-134, higher actinides) for which the inventories are a non-linear function of burnup. It is well understood that the average burnup covers all spatial longitudinal and axial variations of burnup. Spatial variations of inventories at different locations are well known for many radionuclides, however the approach SR 97 does not account for a detailed spatial scenario of water access. The potential inventory based error associated to this approach is probably lower than a factor of 2.

Radionuclide inventories

The total radionuclide inventories appear to be reasonable. The referenced report (Håkanson 1999) is not yet published. However, there is no distinction made between radionuclide inventories in cladding, in fuel matrix and in metal parts. All these inventories appear to be summed up into an overall inventory.

Radionuclide inventories are calculated based on ORIGEN type calculations. This code is validated with respect to major fission products like Cs-137 or Tc-99, as well as for actinides and activation products, however for certain nuclides such as Cl-36 no validation has yet been performed. This is very important as the model calculations of the recent “Spent fuel disposal performance assessment, SPA” project (Baudoin 2000) show Cl-36 to be the dominant dose contributors in many calculations. The quoted uncertainties of 12% for fission products and 20% for actinides are probably realistic for many but are not applicable to all long-lived nuclides. Uncertainties with respect to inventories of Se-79 or of Sn-126 are as high as 600% and calculations for many other radionuclides such as Pd-107 are not yet validated (Guenther, 1991). A large source of uncertainties for inventories of activation products is the impurity levels in the base materials such as Zircaloy, UO_2, Hasteloy etc. This uncertainty could influence the calculated inventories for example of Cl-36 by as much as an order of magnitude. In the performance assessment SPA (Baudoin 2000), the variation of Cl-36 inventories in the sum cladding and structural parts was as high as a factor of 10000 between the assessments of the different project partners ENRESA, VTT, IPSN, GRS, NRG and SCK.CEN. There is no documentation provided in SR 97 which shows how

uncertainties on Cl-36 inventories are considered. A value of $5.5 \cdot 10^8$ Bq/tU was used in SR 97 for the inventory of the sum of fuel rod, cladding and structural parts, which is among the lower values used in the SPA project ($4 \cdot 10^8$-$3 \cdot 10^9$ Bq/tU, variation probably governed by using either maximal allowed impurity levels in the fuel and on the other hand more realistic average inventories of impurities) but no value for structural and cladding parts is given. Instant release fractions of Cl-36 with and without metal parts are equal (6%) indicating insignificant release from structural parts and cladding. Since inventories of cladding and structural parts are considered to be dissolved instantaneously, this would mean that the used inventories for Cl-36 in these metals are extremely small. In the SPA project, the partners were divided in those who assumed that only about 0.01% of the total Cl-36 inventory is in the metal parts and others that considered values as high as 30%. If it were true that as much as 30% of the Cl-36 inventory was in the cladding, than the instant release fraction of Cl-36 in SR 97 would augment by a factor of 6. A recent assessment of radionuclide inventories in the French nuclear energy program indicates an inventory of 2.4 g Cl-36/tU ($2.7 \cdot 10^9$Bg/tU) where about 91% of Cl-36 is in the fuel and 9 % is in structural parts (CNE 1998). Considering this, it appears that the approach of SR 97 is rather optimistic and it is recommended to use higher IRF values for Cl-36 of at least 15% (6% from fuel and 9% from structural parts. It is further recommended to increase the uncertainties in the total Cl-36 inventory to +700%. Using these values in a scenario with large initial canister defects, Cl-36 could become a dominant dose contributing nuclide.

Table 1: Comparison of typical nuclide inventories of SR 97 (Bq/tU) with the range of values used in the European project SPA (Baudoin 2000). SPA data are obtained by various European waste management organizations with burnups between 36 and 55 GWd/tU, with activity values either after discharge or for decay times between 20 and 50 yrs. For comparison, inventories of metal parts and the fuel are added for the SPA data as reported for SR 97

Nuclide	SR97	SPA minimum	SPA maximum
Se-79	2,80E+09	1,60E+10	2,40E+10
Ni-59	8,80E+10	6,00E+10	3,00E+11
C-14	5,00E+10	2,00E+10	9,00E+10
Tc-99	5,70E+11	5,20E+11	7,00E+11
Cs-137	1,80E+15	1,00E+15	5,00E+15
Pd-107	4,90E+09	4,50E+09	7,30E+09
Cl-36	5,50E+08	4,00E+08	3,40E+09
Np-237	1,50E+10	1,70E+10	2,30E+10
Pu-239	9,50E+12	1,30E+13	1,40E+13

A comparison of the used radionuclide inventory with those of the various partners in the European SPA-project is given in the table above for the main nuclides. For many radionuclides there is a close agreement, however, besides Cl-36 another radionuclide

showing large variations is Se-79. The lower Se-79 value at a given fission yield is probably attributed to the larger half-life of about 1 million years used in SR 97, whereas a value of only 64000 years is used in the SPA project (Baudoin 2000). The 6.4E+04 years value is based on the work of Parker (1949), but has been found to contain an arithmetic error of a factor of 10 (O.W. Hermann, 1993) and should at least be 6.4E+05 years, the recommended value of the ENDSF listing from Aug. 2000 is of 1.1 million years is based on the work of Jang et al. (1997) other currently reported values are 0.48E+6 years and 1.13E+6 years. Hence the 1 million year value is more close to the correct value, and the calculated lower activity of Se-79 in SR 97 is more reasonable than the values used in the SPA project.

Inventories of non-radioactive fission products

It appears that non-radioactive fission products such as Xe or the rare earth elements are generally ignored in the description of the fuel and in its interactions with its environment. This has consequences with respect to pressure build-up, fuel microstructure development and radionuclide retention. Rare earth elements provide for example secondary phases that might retain large quantities of trivalent actinides.

Surface area

Fuel BET surface areas between 59 cm^2/g and 121 cm^2/g are reported in SKB 1999b (The quoted particle sizes of 700-1700 mm and 900-1100 mm must be typographic errors, with "µm" being probably the correct value). Spent fuel surface areas are higher than surface areas of unirradiated material, due to accumulation of fission products at grain boundaries. This accumulation makes these grain boundaries more accessible to water. This would mean that surface area is a function of burnup. Thus there is a non-linear coupling between surface area dependent radionuclide release rates and burnup. The report discusses various pros and cons of using BET surface areas. The accessibility of the BET surface area to water has been questioned. Indeed, in the short term of few minutes to hours of a BET sorption measurement it is not certain whether water molecules can enter into all the grain boundaries as easy as inert gases, but it appears reasonable to assume for relevant periods of years to thousands of years that there is sufficient time for water molecules to access the BET surface area. It is not stated which choice of surface area determination (geometric or BET) that is used in SR 97. The reason is probably that fuel surface area is not considered to be one of the major variables in the fuel-cavity-subsystem of SR 97. Indeed, fuel matrix dissolution rates as well as instant release fractions are described independent on surface area in fractional units. However, surface area remains one of the hidden variables in the system because surface area normalized data for the effect of H_2O_2 on unirradiated UO_2 dissolution are used to predict fuel dissolution rates. In case the BET surface area would have been used, the rate would probably be 60 times higher than if the geometric surface area was used.

Representation in SR 97 of heterogeneous radionuclide distribution

For the quantification of the time dependency of radionuclide release it is important to account for the heterogeneous distribution of radionuclides in the fuel rod, i.e. the fuel matrix, grain boundaries, the cladding, the fuel sheath gap and the surfaces of the fractured matrix. This radionuclide distribution depends on fuel type (MOX or UO_2 fuel), irradiation history, linear power and burn-up.

SR 97 points to the increased microstructure and nuclide inventories at the pellet rim, but no consequences are described on how these observations are used in radionuclide release calculations. The highly burned fuel rim contains a few percent of the radionuclide inventory. In SR 97 a very low fuel dissolution rate of 10^{-8}/a is used. The implicit assumption is that this rate is also applicable to the fuel rim, however, there is no discussion at all whether this is reasonable or not. If the porosity is higher, also the local surface area should be higher. This should result in an increase in corrosion rates, and due to the higher radionuclide inventory it should even more result in higher than average radionuclide release rates. Furthermore, higher inventories of alpha-emitters should increase locally radiolytically enhanced fuel dissolution.

Radionuclides in the fuel-clad gap

There is a discussion of literature data on fission gas release, leading to the selection of a reasonable value for gas release of 2% as a reference value, and for Cs release a value of 2% as a pessimistic value. However, a clear analysis, of the expected distribution and of the maximum values is missing. It is stated that the majority of the analyzed fuel has a gas release of less than 5%, without saying whether the analysed fuel is representative for the expected burn-up and linear power distribution. The data indicate that a pessimistic value would lie higher than 5%.

It is confirmed in SR 97 that, in contrast to CANDU fuel, for LWR fuel no systematic study exists on the relation between Cs and I segregation to the fuel clad gap and fission gas release. The few data quoted indicate that Cs release to the fuel clad gap is similar or even higher than gas release. It is therefore probably more coherent to assume that the selected value of 2% for Cs release refers to a reasonable and not to a pessimistic value. The pessimistic value could probably be as high as 5%.

Radionuclide accumulation at grain boundaries, segregation.

It is stated that aside from the ε-Ru-phase the grain boundary inventory is within the margin of error close to zero. Particularly, results from Scanning Auger Analyses of L.Thomas (1988) are quoted to sustain this statement, showing no detectable Cs, Tc and Sr. However the detection limit of this method is close to 1%, and the inventory of Cs in the fuel is 0.4 wt%. Thus, even an accumulation of 2% of the inventory at the grain boundary surface would not be detectable. Fuel powder leach data from the literature indicate that Cs segregation to the grain boundary could amount to values higher than 1%. A reasonable value for Cs is probably close to 1%. In contrast, one can probably

agree that grain boundary inventories of Sr are small. Grain boundary inventories are also discussed in the instant release fractions below.

Long term property evolution of spent fuel in the canister

The properties of the spent fuel are considered in SR 97 to remain identical to its initial state, even though the fuel might be exposed to temperatures close to 200-400 °C for long time periods. Considering the fuel surface temperatures, they may be of equal magnitude compared to those during reactor operation. If the fuel is exposed to such temperatures for long periods, severe property modification cannot be ruled out. It is stated that this is unimportant for post-closure safety because the integrity of the fuel is not threatened. Hence, uncertainties in the initial state of fuel were not considered to be essential enough to be handled in a separate scenario. This is a significant drawback of the present study, considering that in other countries like in France (Poinssot et al. 1999) this is a major research issue. The present database is insufficient to allow conclusion on fuel integrity for times much longer than typical interim storage periods.

It is stated in SR 97 that cladding defects are most likely local, and, due to hydride formation, nonetheless, general cladding failure, though unlikely, cannot be ruled out completely. In the canister defect scenario it is assumed that the cladding has failed locally, but a global failure, with the fuel rod fallen to pieces, has not been considered. For this reason, the radiolysis based fuel dissolution model appears to be based on a hypothetical 100-µm gap between the cladding and the fuel. In addition, criticality calculations appear to be based on the actual geometry of the fuel. There is not only hydride formation to be considered, but also long term irradiation assisted creeping of the cladding due to internal overpressure (He, fission gases) of the fuel rod. This cannot be quantified with the available knowledge, but it adds to the uncertainties of the present approach. The full disintegration of the fuel should be evaluated in sensitivity analyses.

The potential implications of the evolution in fuel structure are discussed in the section on scenario development below.

Environmental conditions relevant to spent fuel performance in a repository

Water composition / redox conditions

Most critical for spent fuel stability, in the presence of groundwater, is the redox state of the water. Groundwater chemistry is not coupled directly into the model chain but is used to determine solubilities of radionuclides and to select relevant property ranges. It is generally assumed that the groundwaters are reducing. However, in the climate

scenario, rather oxidizing environments may also be considered. If these conditions cannot be ruled out, fuel corrosion under oxidizing conditions should be considered as a separate scenario. This will lead to fuel dissolution rates $>10^{-5}$/yr. Alternatively, a statistical evaluation might be useful, showing that it is extremely unlikely to find oxidizing conditions in deep Swedish groundwaters.

It is probably correct that water in the fuel cavities will initially be in the form of vapor. However, if water activity of the vapor approaches unity, condensation might occur. In the case of the canister defect scenario the ingress of groundwater and the subsequent evaporation will lead to the deposition of soluble salts. The presence of these salts might alter the corrosion behavior of metals and of the fuel.

Temperature

Initial fuel surface temperatures are expected to be somewhere between 200 and 400°C. The duration of the high temperature regimes is not given. Uncertainties are considered great. Consequences of high temperatures are particularly important in case of the canister defect scenario, because this could lead to fast fuel oxidation (see below).

Radiation intensity

Since radiation level and dose ratio $\alpha/\beta/\gamma$ are different under disposal conditions compared to those in the laboratory the measured corrosion rates cannot be used directly in performance assessment. The surface dose rate after 40 yrs has been estimated as 700 Gy/h, with contributions by beta radiation to about 15%. These values are more than a factor of 10 lower than respective values calculated in a recent EU-project. Particularly, the value for the beta dose rate appears to be very low. It shall be evaluated what is the reason for these differences and a correct value shall be estimated. The contribution of gamma dose appears to have been ignored.

Calculated dose rate in a container with 4 t of spent fuel (Hauser 1994) are shown in Figure 1 comparing the dose rates for laboratory experiments with a full sized disposal cask (German Pollux cask).

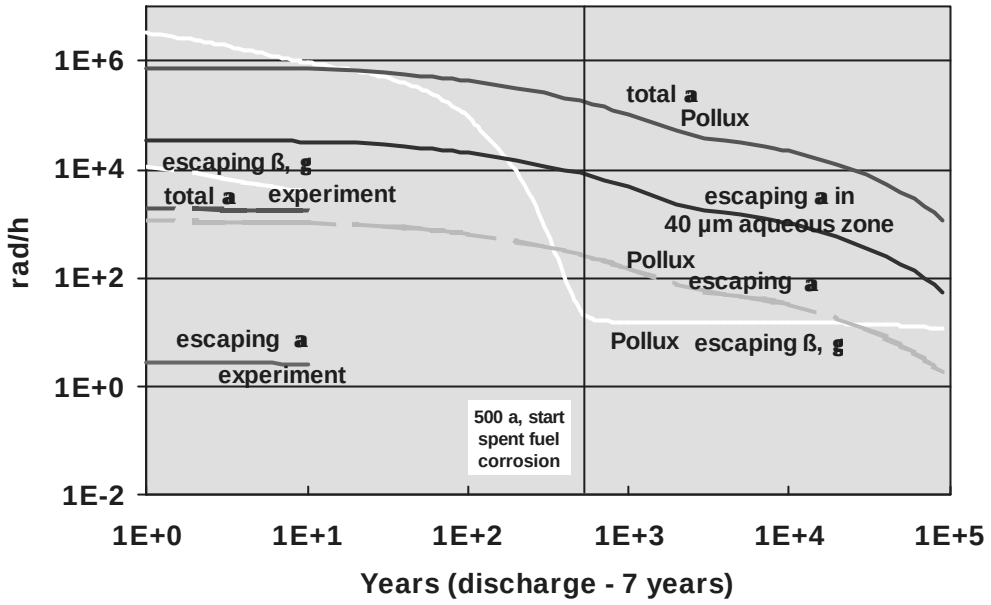

Figure 1: Time dependence of dose rates from spent fuel in experiments (1g in 100 ml solution) and for a water filled Pollux container with 4 tons of fuel. Comparison of dose rates considering the total alpha events with dose rates from alpha events with in an escape depth of 10 µm from beneath the fuel surface. Comparison to hypothetical irradiation of total water volume with irradiation of a volume given by the 40 µm maximum pathway of alpha particles in water

Though the total dose rates expected under disposal conditions are much higher (Figure 1) than in the experiment (both for α and for β,γ) it should be kept in mind, that only a small fraction of α-particles can escape the fuel (19% from 10 µm escape depth) and in the aqueous phase they can only penetrate to a depth of about 30-50 µm. Consequently the α dose rate within this 30-50 µm water layer is the same, both in the experiment and under disposal conditions. After 40 yrs a value of about 400 Sv/h is calculated, a similar order of magnitude as considered in SR 97. In contrast to alpha dose rates, the ß- and γ-rates are much higher than those in the experiments. The reason is the high quantity of fuel in a disposal cask. Beta, gamma dose rates in a SR 97 cask are expected to be about half those in Figure 1, due to the lower quantity of fuel. Differences in SR 97 dose rates and those from the EU project are essentially based on differences in the ß- and γ-dose rates. Maybe these differences are associated to different radiation attenuation in the canister (an iron insert is not present in the Pollux cask).

Gas composition

A water vapor content of about 50 g in a fuel canister is considered to result exclusively from water trapped in the plenum of defected fuel rods. It is stated that about 500 of 1 Mio fuel rods are defective, i.e. 0.05%. Based on about 1100 fuel rods per canister one may agree with the authors that there will be on average less than one defective fuel rod in a given canister. However there will be also a non-negligible probability to find two defective fuel rods in one canister, leading to the double water content in a pessimistic case, which is higher than the maximum permissible water content. Loading strategies of the canisters must therefore ensure that not more than one defective fuel rod is disposed in a single canister. It cannot be excluded that during handling of the disposal container, more than one fuel rod become defective, which will of course not increase the water content.

Also surface sorbed water of at least some atomic layers must be considered. Considering an overall cladding surface in a canister of about 140 m^2, a 1 nm film of surface sorbed water will correspond to 0.14 cm^3. This can indeed be neglected as has been done by SKB. However, there may also be hydrous corrosion products (crud) present on the cladding surface which may release larger quantities of water.

Finally, in the case of defective canister scenario, one may consider a relative humidity of 70% in 1 m^3 void volume, which gives a quantity of 1.5 cm^3 of water. Also this is negligible with respect to 50 cm^3.

For the case of water access to the inside of the canister it is stated in SR 97 that the quantity of hydrogen gas produced by gamma radiolysis will be small in comparison to hydrogen produced by corrosion of the canister. This may not be the case. Experimentally in an EU project with high burnup fuel (50 MWd/kgU) (Grambow et al. 1997) a generation rate of 0.4µg H_2/g fuel/d was observed, corresponding to 300 g H_2/yr for 2 tons of spent fuel. The assumed corrosion rate of the iron insert of 0.1 µm/yr produces on 50 m^2 corroding surface about 1 g H_2/yr. If the iron corrosion rates are really as low as assumed, gamma radiolysis could be a much more important source of H_2 than iron corrosion. It should be noted that in the same spent fuel experiment about 0.1 µmol O_2/g fuel/d were formed, leading in the case of presence of sufficient water to the annual formation of 60 mol O_2/ tons fuel. If this oxygen is used mainly for oxic iron corrosion as expected, the iron corrosion rate will be about 100 times higher than the assumed 0.1 µm/yr.

It is stated in SR 97 that with the small quantity of residual air in a canister only a few mg of nitric acid will be formed by radiolysis. This is probably true for the base scenario but not for the canister defect scenario. Here we need to assume that the inert filling gas has escaped and the free volume of the canister of about 1 m^3 is entirely filled by air. Assuming that 50 g of residual water are in the canister, it could well be that 160 g of nitric acid are formed. The acid will probably react more rapidly with the iron insert than with the spent fuel pellets, leading to a few µm of general corrosion.

It is incorrectly stated that Kr-85 is the main fission gas left at time of deposition. The by far largest fission gas quantity results from non-radioactive Xe. There are about 16 kg of Xe to be expected per canister of which about 3% (500 g, 80 L) can be released instantaneously. This will increase the internal pressure in a fuel rod by about 0.2 MPa. This is probably of no safety hazard. Even if the whole 16 kg would be released in the void space in the canister of about 1 m^3, this will only augment the pressure by 0.27 MPa.

Spent fuel issues in the choice of scenario

Significant scenarios are formulated as a base for the evaluation of the potential evolution of the safety of the repository system. The base scenario considers the thermal, hydraulic and chemical evolution of the disposal system without canister failure and without radionuclide release. Other scenarios are analysed as variations of the base scenario. In the canister defect scenario, a certain quantity of defected canisters is taken into consideration and radionuclide release is evaluated. Other conditions remain the same as in the base scenario. In the base case of the climate scenario the canister remains without failure, but variations of geochemical and hydraulic conditions are considered. The effect of initial canister defects on the climate scenario is considered as a special case. The largest effect of climate on calculated biosphere doses was found for A-berg for interglacial periods, mainly resulting form the effect of changing hydraulic and geochemical conditions on dispersion and radionuclide migration properties. However, it is possible that the scenarios are coupled in a way, that also the fuel dissolution model has to be changed. Consequently, when evaluating the effects of climatic changes within the canister defect scenario it appears necessary also adapt the fuel dissolution model. In some cases, rather oxic conditions are calculated to exist in the climate scenario. If realistic, this could have important consequences on the potential performance of fuel in a defected canister. It is for example rather unlikely that a fuel matrix corrosion rate of 10^{-8}/year will prevail in presence of groundwater oxidants.

Spent fuel related issues in the base scenario

The description includes no single process related to fuel structural alteration. Only radiation induced heat transfer is considered. Even geometric relations inside the canister are considered similar to the initial value. In the base scenario, an important issue could be the potential creep behavior of the cladding due to the effects of gravity and internal pressure built-up. The fuel cladding may break due to creep, hydrogen embrittelment and/or pressure buildup inside of the fuel rod. Important pressure increasing phenomena are fission gas release and generation of He. Significant volumes of He are expected to be generated particularly for MOX fuel, about 6 L per 47 MWd/kgU fuel rod after 10000 yrs (Poinssot et al 1999). Present data do not allow judging the mobility of He in the fuel. If all He would become released to the free void volumes of the fuel rods, 520 bars of pressure would be obtained after 10000 yrs (125

bars for UOX fuel). Much lower pressures are expected if He is retained in the fuel matrix due to slow diffusion.

Moreover, there might be an evolution of the physical state of the fuel (Poinssot et al. 1999). Helium-accumulation and self-irradiation might lead to swelling and also micro-cracking can not be excluded. There might an increase of radionuclide inventories and possibly of He at grain boundaries. Long-term diffusion processes at low temperatures are still difficult to assess. In principal, radionuclide diffusion coefficients are low at T<300°C, but diffusion coefficients may strongly increase due to fuel oxidation. In addition, athermal irradiation assisted diffusion must be taken into account. Accumulation of fission products could lead to a loss of cohesion of the fuel micro-structure.

These processes may eventually lead to a situation were the fuel rod will fail, thus leading to accumulation of fuel pellets at the bottom of the cavities in the iron insert. This could alter radiation attenuation and heat transfer mechanism, leading to vertical temperature gradients at the outer canister surface.

It is today difficult to predict these processes quantitatively. In the base scenario the evolution of the fuel is only relevant for the thermal evolution, because there is no radionuclide release. The heat transfer processes in the canister are assumed to be of influence on the maximum temperature at the canister surface. It is true that the criteria of max 100°C can always been met by appropriate spacing between the canisters, but the uncertainties may be larger than assumed. If the geometric integrity of the fuel rod is disrupted by cladding failure and the rods falls into pieces, the uneven heat distribution at the outer canister surface may locally increase canister surface temperatures. However, since pressure buildup in the fuel rods is a long term process, it is likely that fuel rod failure due to long-term creep is irrelevant for the thermal period in the base scenario and, consequently, the ignorance of these processes in SR 97 is justified for the base scenario.

Spent fuel related issues in the canister defect scenario

Fuel structure modifications prior to water access

In SR 97, the structural integrity of the fuel is considered to remain unchanged. However this is not the most likely case for a scenario with defective canisters. In this case it is possible that oxygen enters the canister already years before the canister is disposed. The effect of a presence of oxygen is not discussed in SR 97. Considering the initially high fuel surface temperatures during storage and disposal fuel oxidation is expected to take place, provided that the cladding is defect. A detailed study about this is given by Hanson (1998). Oxidation of the fuel initially leads to the formation of U_4O_9, associated to a reduction in specific fuel volumes. The oxidation is more rapidly along grain boundaries. This leads to formation of U_4O_9 oxidation rims along all grain boundaries (Thomas et al.1991). The volume reduction makes the grain boundaries more accessible to subsequent leach processes. Oxidation of spent fuel to $UO_{2.4}$ occurs

relatively fast, for example it takes only about 2 years at 175°C (Hanson 1998). If the oxidation goes beyond an oxygen to metal ratio (O/M-ratio) of about 2.42, U_3O_8 forms. This phase is about 20% less dense than UO_2. The increase in volume causes fuel expansion and establishes stresses on the cladding which will split as a result (Hanson 1998). U_3O_8 has also a higher dissolution rate than UO_2. Hence, faster radionuclide release might be expected to occur with oxidized spent fuel. The rate of oxidation of $UO_{2.4}$ to U_3O_8 depends both on burnup and temperature. According to previous observations (Einziger and Strain 1986), spallation of fuel fragments due to volume increase takes less than 3 h at 360°C and less than 5000 h at 250°C. It is clear that 5000 h is a very short period in a defected container. One can conclude from this that a transformation to U_3O_8 of failed fuel rods is likely to occur in defected oxygen containing canister for the temperature range of 200-400°C. This could lead to much earlier cladding failure than in the base scenario in SR 97. This has not only consequences for canister surface temperatures as discussed above for the base scenario, but also for the criticality calculations that are based on initial emplacement geometry. Potential changes due to mechanical cladding failure have not been considered in SR 97.

Concerning radionuclide retention one can conclude for the canister defect scenario that data on the leaching behavior of oxidized fuel are as relevant as those of non-oxidized fuel. Leach data using oxidized fuel are scarce in the literature. All leach tests with oxidized fuel have been performed under oxidizing conditions. These data (Gray 1998) show an increase in surface area normalized matrix dissolution rates of oxidized spent fuel (U_4O_{9+x}) by as much as a factor of 6. Moreover, due to fuel oxidation, the quantity of accessible grain boundary surface area increased by as much as a factor of 10. The combined effect of surface area increase and increase in matrix dissolution rates was as high as a factor of 10. However, it needs to be mentioned that these rates are not applicable to repositories under reducing conditions, here U_3O_8 or U_4O_9 might be thermodynamically unstable and might be transformed back to UO_2. No data exists to estimate whether this would lead to an increase or to a decrease in fuel dissolution rates.

Water intrusion

The processes of water intrusion into a defected canister appear to be described qualitatively correctly. The effect of water transport via vapor phase appears to deserve a more quantitative treatment. Particularly, it is unlikely that the inward diffusion of water vapor gradually will approach a mass transfer rate of zero. The diffusion rate is governed by the diffusion length (the depth of the defect, which is constant) and the partial pressure difference between the inside and the outside, which asymptotically reaches a constant non-zero value. This value is governed by a constant water activity at the outer canister surface and a steady state between water vapor consumption and inward diffusion.

Also it appears that the role of slow water diffusion in the bentonite is overestimated as a limiting factor. If, as stated, the water enters initially into the canister by an advective process (driven by 5-7 MPa of pressure difference between the inside and the outside), in the absence of diffusion limitations in the bentonite, even a small hole of 1 mm^2

could at a rapid rate fill the canister with water. This would occur a long time before the build-up of a hydrogen pressure counteracts water ingress. Water transfer from the bentonite to the canister would probably lead to a partial desaturation of the inside bentonite surface. Resaturation by external groundwater is an advective and not a diffusive process. Hence, advective transport of water in the bentonite may play a much larger role than anticipated.

The irradiation of water leads not only to the formation of water radiolysis products, but also to a higher concentration of dissolved salts in the canister. This effect is of course of minor importance in the time frame of thousands years, but it could be important if the water is irradiated or consumed by corrosion close to dryness.

Redox conditions in connection with water ingress

The radiolytic effect on redox conditions is correctly described, but this description is very general. There is no detailed evaluation of neither the dominant radiolytic reactions and their corresponding rate constants, nor of the mass transfer processes (H_2 diffusion, water exchange, U-release) between the fuel-cladding gap and the external water.

Radionuclide release from spent fuel

The radionuclide release model (source term model) for spent fuel is based on fuel with current properties, with the exception of the radiation fields. Fuel property evolutions prior to water access are not considered even though these processes might alter radionuclide release characteristics as discussed above.

The SR 97 approach appears to be based on the conviction that a direct prediction of long-term behavior of spent fuel from laboratory experience and laboratory based models is not possible. The reason behind this conviction is that radiation plays a large role in fuel stability and that the radiation fields of recently discharged fuels are much higher than expected in the repository. The spent fuel performance and its role in the multibarrier system is therefore assessed by a systems approach, passing from mechanistic interpretation of surface reactions of unirradiated and irradiated UO_2 via radiolytical modeling and conservative simplifications to source term quantification. Radionuclide release from the fuel rod is described by only two terms, the instant release fraction and the fuel matrix dissolution rate.

In the following, the quantification of fuel matrix dissolution rates is first discussed and after that the instant release fractions. Finally, the quantitative distribution between the two terms is evaluated. Special intention is given to the role of grain boundary release.

Model for the release of matrix bound activity

The fuel dissolution and release of radionuclides under anoxic conditions is described as if uranium dioxide is the dissolving phase, whose dissolution is a prerequisite for the release of radionuclides bound into the solid solution of the UO_2 matrix. It is true that the matrix of spent nuclear fuel to a large extent resembles the structure of the unirradiated UO_2. However, due to defect accumulation and incorporation of fission products and actinides in the UO_2 matrix, the population of surface sites with bond strength different from that of pure UO_2, the properties will not at all be the same in unirradiated and irradiated material. Hence, both corrosion rates as well as solubilities might be different for irradiated and unirradiated material.

The results found in the literature on the effect of oxidant concentrations on corrosion rates are nevertheless essential for the understanding of spent fuel performance because this effect is more difficult to investigate with real spent fuel due the self-oxidation by radiolysis. Controversial oxidant concentration dependencies have been reported, with reaction orders varying between 0 to 1. When the dissolution rate is determined at the beginning of the experiment, the dependence of the oxidant concentration corresponds to a reaction order of 1. In salt brines, a linear relationship has been found for the three different oxidants: O_2, H_2O_2 and ClO^- (Giménez et al. 1996). The same dependence was obtained in electrochemical experiments (Shoesmith et al. 1992).

Fuel matrix dissolution rates

Based on modeling as well as on experimental data of non irradiated UO_2 dissolution under reducing conditions, it is suggested by SKB to use a constant fuel matrix dissolution rate of 10^{-8}/a as a reasonable value. It is surprising not to find a single rate value from Swedish experiments with spent fuel in SR 97. It is stated that a pessimistic value cannot be given. This approach is based on a discussion both of a solubility based model and a model for radiolytically enhanced fuel dissolution.

Solubility limited model

The *solubility based model* is not used to quantify radionuclide release in SR 97 but it is used only in an indirect way as a background condition for the radiolysis model. Indeed, a solubility limited model is only valid in the absence of oxidants. In a reducing geochemical environment, radiolysis is the only source of oxidants. Hence, the solubility based model is the base for the justification of the radiolysis model.

The solubility based model is described in SR 97 as if UO_2 is the dissolving phase. Such model is only valid if UO_2 is the dissolving phase and if no other more stable phase is formed as a secondary alteration product. The spent fuel matrix is similar to UO_2 but there are large differences, mainly related to impurity contents. The solubility of UO_2 in reducing groundwaters lies between 10^{-9} and 10^{-10} mol/l. A value of $1.3 \cdot 10^{-7}$ mol/l is used in SR 97 as recommended by Bruno et al. (1997). However this may be an upper limit. Experimental data with spent fuel exposed to reducing conditions in the presence

of metallic iron (Grambow et al. 2000) or in the presence of H_2 (Spahiu et. al. 1999) yield solubilities in the order of 10^{-8} mol/l at 25°C. It is not clear whether the observed 10^{-7}-10^{-8} mol/l have any bearing with the solubility of the dissolving matrix. The presence of trace elements and surface energy could increase the solubility. It could also not be excluded that the solubility is enhanced by effects of radiolysis, stabilizing certain steady state concentrations of dissolved uranium (VI) species. In case of radiolysis one might expect reprecipitation of UO_2 at some distance of the radiation source. This could lead to the coprecipitation of radionuclides with UO_2. In contrast, if solubility is enhanced due to surface energy or due to the presence of trace elements, the difference between the solubility of UO_2 and that of the spent fuel matrix of more than a factor 100 could cause a driving force for fuel dissolution: precipitation of pure UO_2 with a solubility of 10^{-9} mol/l may allow spent fuel to dissolve continuously. This mechanism cannot be ruled out if the conceptual model of higher solubilities of spent fuel versus UO_2 is retained.

Model with radiolytic oxidation

The *radiolysis model* is evaluated in detail in the Appendix. The radiolysis calculations of Eriksen are quoted in SR 97 without going into details. The conclusion of Eriksen is that H_2O_2 is the principal oxidant and that the formation of radiolytic H_2 counteracts the oxidizing effect. The effect of H_2O_2 in accelerating UO_2 dissolution is well known. However, whether oxidation by H_2O_2 is rate determining or whether other oxidants or radicals are more important remains to be demonstrated. The effect of H_2 is also demonstrated experimentally, but it is not yet clear how this effect can be quantified in a model. The presented model will yield very low rates at high H_2 pressures, but there are no experimental data to sustain these low fuel dissolution rates.

The model is based on irradiation of a 100µm water film in between the fuel and the cladding. This assumption is only valid if the cladding remains attached. The validity of this assumption is not evaluated in SR 97. Diffusion processes as well as advection due to gas bubble formation in the 100 µm are ignored. About 40 chemical reactions of radiolytic species in water are used to describe the system (see Table 1, Appendix). The validation of this system of reactions is difficult. Even for deionized water differences between calculated and experimental production rates of radiolysis gases were as high as a factor of 10 (Grambow et al. 2000). It appears that even in deionized water, uncertainties are extremely high. Even more difficult is the assessment of the effect of groundwater composition. Effects of ionic strength and water composition are often difficult to account for. The effect of parameter uncertainty on results of the calculations has not been assessed. The presence of certain trace elements (Br etc.) or of redox sensitive surfaces may strongly alter the results of calculations. This is also true for the effect of dissolved Fe(II) species, for the presence of chloride ions (formation of hypochlorite) etc. If applied to the thin film of water between the cladding and the fuel, also the effect of dissolved Cs and of the potentially high pH values needs to be considered. None of these difficulties are addressed in SR 97.

Only the reaction of molecular oxidants H_2O_2 and O_2 with the fuel are considered in the SR 97 model. However, reaction rates with radicals are expected to be much more

rapid. Even if the concentration of radicals is much lower than that of molecular species, they might contribute significantly to overall reaction rates. Also radicals are precursors of molecular species. If they react with the fuel, less molecular species are formed. This effect is difficult to quantify. Attempts have been made previously by Christensen (1999) to explicitly account for these reactions. This involves the adaptation of various surface reaction rate constants to experimental data, an approach that is difficult to validate.

In SR 97 the spent fuel reaction rate is in principal proportional to the concentration of H_2O_2 in solution. Assuming that H_2O_2 is indeed the rate determining species, there are secondary rate controls than just a direct concentration dependency in terms of a surface reaction. In the Appendix, the Eriksen model (SR 97) is applied to deionized water and is compared with the results obtained by using the model of Christensen (1997) for the same experimental conditions. Long term fuel dissolution rates were found to be more than 4 orders of magnitude faster when using the Christensen model compared to those from the model of Eriksen. This difference could be attributed to differences in the model for radiolytic and non-radiolytic decomposition of H_2O_2.

Rates could also become dependent on the availability of H_2O_2 if solution concentrations are very low. In other words, it cannot be ruled out that, at low oxidant concentrations, the spent fuel surface reacts with any H_2O_2 specie that hits the surface. This implies that the radiolytic surface could become influenced by transport phenomena, hence, transport of H_2O_2 to the surface is slower than the reactive consumption of H_2O_2.

It is stated in SR 97 that our fundamental understanding of the processes of water radiolysis is sufficient and that there are no fundamental uncertainties relevant to safety assessment. We may conclude from the above arguments and from the evaluation in the Appendix that this is not true, neither for the irradiation of deionized water nor for typical ground waters. Today, the present radiolysis models are useful to explain experimental data. However, neither the radiolysis/H_2O_2 model of SR 97 nor the model of Christensen is validated to allow for reasonable predictions to be made.

Coupling of the solubility and the radiolysis model

The coupling of the radiolysis model and the solubility model is not discussed in SR 97. Both models can be considered as representing two parallel reaction branches, among which the fastest is controlling the overall release rate. If radiolysis is faster than solubility limited release, radiolysis is rate controlling. In the European project SPA (Baudoin 2000) the participant "ENRESA" developed this coupling in an alternative source term model considering not only solubility and advective flow but also the diffusive mass transfer resistance of the bentonite buffer material. Using a solubility value of $5 \cdot 10^{-7}$ M for UO_2(fuel), this work has led to the conclusion that the radiolysis model would yield faster release than solubility controlled release for time periods of 1 Mio yrs. If solubilities are lower (than $5 10^{-7}$ M) as can be expected, the solubility limited release model will yield extremely low mass transfer rates, justifying the radiolysis model as the dominant release model for safety relevant time periods.

Extrapolation of a value of the matrix dissolution rate from experimental data

The reaction rate of 10-8/yr (assumed to represent a reasonable case) is calculated using the radiolysis model. This rate is orders of magnitude lower than everything ever measured with real spent fuel, including tests performed under reducing conditions and including tests with non-irradiated UO_2. No rate constants or other data are provided in SR 97 that would allow a reader to evaluate the quantification procedure of this rate. One is referred to unpublished calculation results. In the following the extrapolation procedure is therefore only discussed in a qualitative and not in a quantitative fashion.

After the prediction of molecular oxidant (H_2O_2, O_2) concentrations with the radiolysis model, rate data for the reactions between UO_2 and molecular oxidants are used to predict fuel dissolution rates. There is no experimental proof that the reaction rates of H_2O_2 with UO_2 and with spent fuel are the same. In particular, it must be accounted for that the rates of UO_2 dissolution in presence of H_2O_2 are directly proportional to surface area, since specific surface areas of spent fuel and UO_2 are different. Application of reaction rates of UO_2 to spent fuel is highly uncertain due to surface area dependence. No specific surface area is given in SR 97.

The experimental reaction rates between H_2O_2 and UO_2 vary by as much as a factor of 10. Considering this, the reaction order between H_2O_2 and UO_2 can only be determined with a high degree of uncertainty. As acknowledged in SR 97 the relation between H_2O_2 concentration and reaction rates is extrapolated to very low H_2O_2 concentrations, i.e. for conditions where no experimental data exists. Lowest H_2O_2 concentrations employed experimentally are about 10^{-5} M. This is very high when extrapolated to long time periods. The mechanism of interaction is not sufficiently well understood to allow such an extrapolation. This is indicated by the discussion of the authors of SR 97 by acknowledging the potential variation in the exponent of the rate law (reaction order).

Chemical dissolution rates of spent fuel in the hypothetical absence of radiolysis under reducing conditions

In the absence of radiolysis and other oxidants, the corrosion rate is not necessarily governed by the thermodynamic solubility of the dissolving fuel matrix and the mass transfer of dissolved uranium species by diffusive and advective processes. These rates are extremely low, due to the low apparent diffusivities of U(IV) in the bentonite buffer and the low solubility in the fuel cavity. Faster rates could be obtained, if initially dissolved U(IV) is sorbed or precipitated on canister material or its corrosion products. This consumption of uranium from solution could act as a pump for the continued dissolution of spent fuel. Indeed, precipitation of UO_2 has been observed on metallic iron (Giménez et al. 1998). Moreover, in silica rich groundwaters, coffinite ($USiO_4$) is more stable than UO_2. Natural analogue data indicate release of trace elements (lanthanides) upon coffinitization of UO_2 (Janacek et al. 1992). Under these circumstances the release rate of radionuclides may be governed by the rate of coffinitization of UO_2. This rate in turn will depend on the supply of silica from the ground water and/or on the growth rate constants of coffinite crystals. The latter will depend strongly on temperature. Similarly as discussed for coffinitization, there may also be sorption, coprecipitation or precipitation of Uranium (IV) on the canister or

canister corrosion products. UO_2 precipitation on metallic iron from U(VI) containing solutions (Giménez et al. 1998), sorption and coprecipitation (Grambow et al. 1996) of both U(VI) and U(IV) on corrosion products (magnetite) have been observed experimentally. The thermodynamic driving force imposed on spent fuel dissolution has not yet been quantified.

Geochemical constraints on fuel matrix dissolution rates

The fuel matrix dissolution rates in SR 97 appear to be considered to be independent of temperature and geochemical variables such as pH, pCO_2, Eh. The only condition considered appears to be the assumption of overall reducing conditions. This approach may be valid in part for recently discharged fuel with high radiation fields. Radiolysis can mask effects of temperature, pH, Eh and pCO_2. This can be shown by a comparison of spent fuel leach data with those of unirradiated UO_2. However, data for dissolution rates of UO_2 and of spent fuel under oxidizing conditions seems to indicate that the major difference is the specific surface area. Such an investigation has not yet been conducted for reducing conditions. Here corrosion rates of spent fuel are much higher than those of UO_2, due to radiolysis effects. It is difficult to distinguish between radiolysis effects and higher reactivity of surface sites. Nevertheless, such distinction is necessary for a model of spent fuel dissolution based on the behaviors of unirradiated UO_2.

The schematics of the masking effect of radiolysis are illustrated by Figure 2. There is probably a critical concentration or a critical temperature below which spent fuel properties in contrast to UO_2 properties become independent on these geochemical variables. If a particular geochemical parameter value would lead to rates of UO_2 dissolution higher than those of irradiation assisted dissolution of spent fuel, a corresponding increase in spent fuel corrosion rates might be expected. The more the radiation decays the lower the rates become, and consequently the lower is the critical temperature or critical concentration. Thus, the more important are these variables as controls of the dissolution rate. There is a relationship between the reaction order of UO_2 dissolution rates and other environmental variables apart from radiation. It is not yet possible to account for the potential environmental effects on fuel corrosion rates under reducing conditions, but from data of unirradiated UO_2 it is clear that a model only based on radiolytic oxidant concentrations such as the one proposed in SR 97 is insufficient. Certain observations are illustrated in the following:

Temperature: The effect of temperature on the oxidative dissolution process of unirradiated UO_2 suggests activation energy values between 20 - 60 kJ mol^{-1} (Gray et al. 1992, Grandstaff et al. 1976, Hiskey 1979, Aronson et al. 1957). De Pablo et al. (1997) have performed dissolution experiments as a function of temperature. The apparent activation energy calculated was 49.5 ± 16 kJ mol^{-1} in the range between 10 – 60 ºC, This value is much higher than the value determined with spent fuel (Gray et al. 1992). Leaching experiments performed with spent fuel under oxidizing conditions have shown no differences on radionuclide release at temperatures lower than 150 ºC. However, an effect of temperature was observed at higher temperatures.

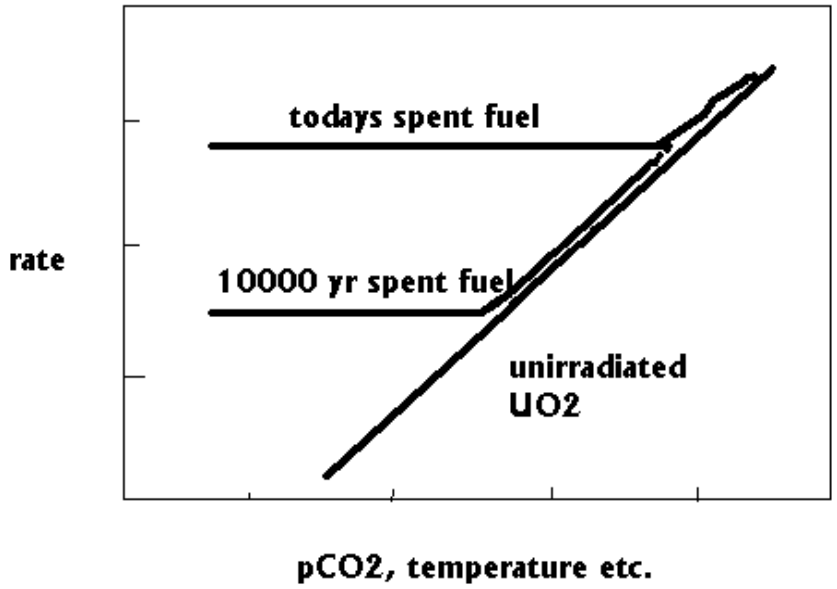

Figure 2: Schematic illustration of the effect of geochemical variables on the comparison of the rates of unirradiated UO_2 with that of spent fuel.

pCO_2: Carbonate is present in all granite groundwaters to a major or minor extent. Therefore, several authors (Gray et al. 1992, Gray et al. 1995, De Pablo et al. 1997, Posey-Dowty et al 1987, Grandstaff 1976) have studied the effect of carbonate on the dissolution rate. Although some discrepancies related to the reaction order have been found in the literature, most of the experiments performed at 25 ºC indicate a fractional reaction order equal to 0.60. In a recent European project (Grambow et al. 2000) corrosion rates of spent fuel were found to be independent of pH and pCO_2 in the studied range whereas, under similar conditions for unirradiated UO_2, a dependency of corrosion rates on carbonate was found. The insensitivity of spent fuel to these geochemical parameters is explained by rate control by radiolytic oxidants.

Redox: Experiments performed in the 3rd Framework programme of the EC show that spent fuel corrosion can be about two orders of magnitudes faster than dissolution of unirradiated UO_2 (Grambow et al. 1997). However, under strong overpressures of O_2, as well as in carbonate solutions, the reaction rates are similar. Radioactivity is not the only explanation for this difference. Other explanations include effective surface area, defect structure, fission product accumulation at grain boundaries etc.

pH-dependency: Torrero et al. (1997) studied dissolution rates as a combined function of both pH and oxygen partial pressure. Data treatment showed that the dependency on proton concentrations follows fractional reaction orders. For pH values between 3 and 6.7 a reaction order of 0.37 was obtained while at higher pH no such pH dependency was observed. At acid pH, for the oxygen partial pressure dependency, the reaction order has been found to be 0.31, while at basic pH, this dependency can be considered negligible. Regarding the fractional order dependency with respect to proton concentration, Torrero et al. (1997) as well as Thomas and Till (Thomas et al. 1984)

obtained similar results. A recalculation with their data has given a value of 0.30 between pH 2 and 5 (Grambow et al. 2000).

Since it is today impossible to sufficiently accurately quantify the above described effects for old spent fuel with low radiation fields, it is necessary to consider the dependency on geochemical variables within the parameter uncertainty.

A pessimistic fuel matrix dissolution rate

It is correctly stated in SR 97 that the assumption of a first order concentration dependence of reaction rates on H_2O_2 concentrations may result in significant underestimation of the reaction rates for the conditions of the expected low oxidant concentrations in a repository. It is also stated that measurement uncertainties do not allow measurements in the relevant low oxidant concentration range. It was correctly concluded to consider this as conceptual model uncertainty. However, this is in conflict with the rejection of the choice of a pessimistic matrix dissolution rate. Considering the large model uncertainty for detailed radiolysis calculations it appears questionable whether a "reasonable" matrix corrosion rate can be given at all. It appears simpler to give a pessimistic bounding value than a reasonable value.

It is argued by SKB that the use of a pessimistic value would be identical of an "instant coffee" dissolution model. This is not necessarily the case. There is not only the alternative between instant release and release within a period of 100 million years. Pessimistic bounding values can be identified, which consider both conservative data interpretation and model choices as well as uncertainties in data, models and scenarios without being overconservative. The boundary between a robust conservative approach and an overconservative approach may be discussed in the light of spent fuel leach data.

A pessimistic but not overconservative rate could either be determined from experimental data of spent fuel corrosion or from conservative models. A maximal empirical rate could be obtained from experiments performed under oxidizing conditions. Initial rates under oxidizing conditions are very high (10^{-3}/yr) but it would be overconservative to use these rates as a bounding case because the rates decrease with time to a limiting value of about 10^{-5}/yr. This long term rate of fuel matrix dissolution was also measured (Forsyth 1995) in the STUDSVIK laboratory for dissolution under oxidizing conditions in Swedish groundwaters. Even this rate is overconservative because the rates of corrosion under reducing conditions will be lower. Under conditions of overall reducing groundwaters, the decay of radiation sources will finally lead to a decrease in reaction rates. However, a simple extrapolation of the radioactive decay effect to very low rates is definitely neither conservative nor realistic. The rate cannot approach zero. Various boundary conditions may be considered. There does not exist a sufficient experimental database for reducing groundwater conditions to allow for the derivation of a low reasonable value of the matrix corrosion rate. The lowest rates measured are encountered in recent tests with partial pressures of hydrogen of 2.7 bar, generated by Fe corrosion. Spent fuel corrosion rates were lower by at least a factor of 500 when compared to tests under oxidizing conditions. Long-term dissolution rates were close to the detection limit, given by a rate of about 10^{-9}/d (Grambow et al.

2000). Very low reaction rates were also observed in well controlled spent fuel powder dissolution tests (Spahiu et al. 1999), using 5 MPa of H_2 overpressure, but maximum values for fuel corrosion rates has not yet been derived from these data. In contrast, a large international and Swedish experimental database exists, which shows that reaction rates could be much larger under reducing conditions.

Summary of uncertainties in fuel matrix behavior

In conclusion, it must be disagreed that there are no real uncertainties in the basic understanding of fuel matrix dissolution. In the literature, fundamental model uncertainties persists: current models include (1) alpha radiolytic assisted dissolution, (2) beta radiolytic assisted dissolution, (3) chemical dissolution under reducing conditions, caused by mass transfer between various U(IV) solid phases, (4) surface complexation etc. All of these models have not yet been tested for their predictive capacities.

The simplification by a constant rate seems to be reasonable but the comparison with a case where the barrier function of spent fuel is entirely ignored appears to be excessively conservative. The real uncertainty in long-term rates varies not between "instant coffee" dissolution and corrosion rates of 10^{-8}/yr but between 10^{-9} and 10^{-5}/yr. In a recent EU-project (Grambow et al. 2000), it was concluded that in the presence of iron or other reducing species anticipated for most repository designs, corrosion rates are expected to remain lower than 10^{-6}/yr.

Instant release fractions

The release from fracture surfaces and the fuel cladding gap comprises a significant fraction of overall radioactivity release from the fuel and, due to its high mobility is considered as an instant release fraction (IRF).

Grain boundary release is not accounted for specifically. There is also no specific consideration for release from structural parts of the fuel assembly. In order to cover releases from grain boundaries, from cladding and from structural parts, the entire inventories associated with these releases are considered to be part of the instant release fraction. It is clear to the authors of SR 97, that this approach is a large simplification. Release form structural parts as well as from the cladding may take many 1000 of years. The ignorance of these kinetics releases is justified in the context of a conservative approach. However, this is incoherent with the strategy of SR 97, which attempts to give both pessimistic and realistic estimates.

The approach is also justified in case that the expected metal dissolution kinetics is fast in relation to subsequent transport processes. This may be the case for a rather late water access scenario, but slow release kinetics from metal parts may serve as an important barrier in the case of early water access. The effect on overall safety will be small if only small quantities of long-lived radionuclides are concerned, but the results of SR 97

calculations show that activation products such as Ni-59 (almost entirely contained in metal parts) are one of the major dose contributors. Uncertainties with respect to Cl-36 inventories are large, thus even Cl-36 could become a dominant nuclide challenging the overall repository safety. Considering these nuclides as instantly released is conservative (if inventories are correct) but a more realistic calculation would also be useful. In the recent approach of the European project "SPA" (Baudoin et al 2000) release from cladding and structural parts was considered with a constant rate of 10^{-3}/yr. There are a lot of uncertain assumptions related to the dissolution rates of these metals. Considering a 10-fold increase in dissolution rate did only change maximal doses from the repository slightly, indicating that a total dissolution period of 1000 yrs is almost the same as an instant release. A decrease in metal dissolution rates by a factor of 10 decreased maximal doses by about a factor of 2. Considering the uncertainties involved, the small effect on long term doses and the efforts necessary to sustain a very low metal dissolution rate, the approach of SR 97 is reasonable with radionuclides in cladding and structural parts included in the instant release fraction.

IRF values depend mainly on burn-up and linear power rating (Stroes-Gascoyne 1992). The instant release fraction in SR 97 comprises also the much slower release of radionuclide inventories from grain boundaries as well as from metal parts. Essentially all radionuclide sources with release rates faster than the matrix are considered to be released instantaneously. This is of course form the point of view of the conceptional model a pessimistic and possibly over-conservative assumption.

Nevertheless, grain boundary inventories are not very well known. Based on fission gas release data as well as on fuel leaching data for CANDU as well as fuel LWR fuel both reasonable as well as pessimistic values for instant release fractions (IRF) were identified. The list of data in SR 97 is compared with those used in the SPA project (Baudoin 2000).

Large differences in the IRF values of SPA and SR 97 are associated to the explicit source term for metal parts in SPA, the different consideration of the contribution of the ε-phase to instant release and the omission of recoil phenomena in SR 97. A certain quantity of actinides is implanted into the fuel cladding by alpha recoil phenomena to a depth of a few tens of nm. Assuming a penetration depth of recoil nuclides of 50 nm, this would amount to an actinide inventory fraction of about 0.001 % in the cladding. In the same way, but to a larger extent of about 0.1% by fission recoil, fission products are incorporated into the inner fuel cladding surface to a depth <10 µm. A certain fraction of this may be easily accessible. The values of 0.5% used in the SPA project appears to be overconservative.

Table 2: Comparison of reasonable estimates and pessimistic IRF values in SR 97 and in the SPA project (Baudoin 2000).

	SPA	SR97 reasonable	SR97 + metal parts	SR97 pessimistic
Cs-137	5	3	3	6
I-129	5	3	3	6
Rh	5	-	-	-
Zr-93	5	-	-	-
Cl-36	5	6	6	12
Tc-99	2	0,2	0,2	1
Pd-107	2	0,2	0,2	1
Sn-126	2	2	2	4
C-14	2	5	15	55
Se-79	1	3	3	6
Ag-108m	-	3	100	100
Actinides	0,5	-	-	-
Ni-59	0,5	-	100	100

The contribution of the ε-phases and particularly of its Tc content to the instant release fraction deserves a special attention. The proportion of accessible ε-phases in grain boundaries is unknown. Recently it was shown that 2% of the total Tc inventory of the fuel could be released from grain boundaries within 5 years (Finch et al. 1999). Grain boundary inventories are probably even higher. Grain boundary inventories are, from the conceptual model point of view independent on the water access scenario. Following the logic of SR 97, they must be included into the instant release fraction, if their release rates are higher than 10^{-8}/yr. Nevertheless, based on leach data it is argued in SR 97 that IRF values of Tc are lower under reducing than under oxidizing conditions. Lower Tc release under reducing conditions can be attributed to solubility controls for Tc(IV). Conceptually it appears more reasonable to keep the instant release fraction on its value for oxidizing conditions and consider low Tc release subsequently by the coupling of the source term to solubility. In the same way it is argued that the IRF values increase with increasing temperature for C-14 and I-129. Even if finally pessimistic values are chosen, it looks like the IRF values are in some cases used as a fudge factor that comprise all types of empirically observed high initial release. There seems to be a lot of subjective judgement involved in the chosen IRF values. An example is quoted from SR 97: *"Regarding C-14, Antillia (1992) suggests that the inventory is shared between the fuel (50%), the cladding (40%) and the metal parts (10%). Given the durability of the cladding it seems reasonable to only add another 10% IRF for C-14 as a reasonable value but assume another 50% as a pessimistic value. "* Why follow the suggestions of Antilia (1992)? Can they be generalised? Inventories in cladding and fuel as well as in structural materials could be calculated with more accuracy using actual impurity levels in the non-irradiated UO_2, metals as well as in the cladding. The base of only using 10% not 50% of the inventory in the reasonable IRF implies form the point of view of the overall release model (total release = IRF + fuel matrix dissolution rate) that the residual part in the cladding is released with the rate of fuel matrix dissolution i.e. by 10^{-8}/a. This seems to be optimistic without a clear technical base.

It is stated that the corrosion rate of Zircaloy and the release rate of activation products is governed by the solubility of ZrO_2 which is very low (10^{-9} M). However, the chemistry of dissolved Zr is only poorly known and the utilized solubility calculations are associated with uncertainties of many orders of magnitudes. Furthermore, the proposed solubility controlled mechanism assumes that there is no radionuclide release from the Zr-oxide film, for example by diffusion processes. Until now there does not exist a single experiment worldwide which shows that radionuclide release rates are controlled by the solubility of ZrO_2. Furthermore, it has not been considered that the radionuclides are unevenly distributed in the cladding. Radionuclides implanted by recoil mechanism in the fuel cladding are only concentrated on the inside surface to a few nm (alpha recoil nuclides) or µm (fission recoil nuclides) of depth.

Corrosion of the cast iron insert

It is stated that corrosion rate of Ni-based alloys is about one µm/yr and the corresponding rate of stainless steel corrosion is tens of microns. With these corrosion rates it is surprising that the corrosion rate of the cast iron insert is only 0.1 µm/yr.

The exclusive consideration of magnetite seems questionable. Radiolytic oxidants are expected to produce, depending on the temperature, either hematite or goethite. At low temperatures, the formation of magnetite is not confirmed experimentally. The selected low corrosion rates of iron under anaerobic conditions are based on the formation of a protective magnetite barrier. The formation of magnetite depends on temperature. In the description of iron corrosion, aerobic corrosion is entirely missing. However, aerobic corrosion mechanisms are probably dominant during radiolytic enhanced iron corrosion. The observed maximum corrosion rates under anoxic conditions will produce about 66 dm^3 H_2/year under anaerobic conditions (the equation 3 on page 75 in SKB 1999b is not charge balanced). In contrast, more than 1 m^3/ year is expected to be caused by radiolysis. This shows that at least under anoxic conditions, radiolytic enhanced iron corrosion will be much more important than that of anaerobic corrosion. Radiolytic iron corrosion is based essentially on the gamma dose. As such, an evaluation of this effect would require that the time of initial water access to the canister interior is considered. It is after all surprising that radiolytic iron corrosion is not considered in SR 97. This is an important drawback, as it may also influence scenario development: Radiolytic iron corrosion may lead to critical gas pressures of 14 bars in the canister within as little as 10 years, much earlier than that predicted based on slow iron corrosion. This could make disruptive H_2 release through the bentonite barrier to become more likely to occur and more frequent.

Chemical evolution

The analysis of canister corrosion is characterized by processes that occur in the absence of oxygen. The arguments used to prove the absence of oxygen at repository horizon for all times are essentially valid for all sites of similar depth. It would therefore be useful to provide a statistical evaluation, showing that the infiltration of oxygen containing recharge waters will never lead to oxidation processes at repository horizons.

Concerning canister corrosion, only an incomplete assessment of the effect of sulfides is given. It needs to be evaluated, whether a coupling of the iron(II)sulfide and Cu-sulfide system will clarify the picture. The assessment of corrosion effects is based on thermodynamic equilibrium of the Cu-base metal with its environment. This review recommends that SKB perform a detailed evaluation as to whether a particular assessment of the corrosion behavior of welds or heat affected adjacent zones is necessary. It shall also be evaluated whether Fe-Cu mixed oxides or sulfides might disturb thermodynamic equilibria.

References

Antilla M., “Spent Fuel Characteristics for TVO-92 safety analysis”, Helsinki, Nuclear Waste Commission of Finnish Power Companies, Report YJT-92-03, quoted by SKB report TR-99-09 (1999)

Aronson S., Roof Jr. R.B. and Belle J. (1957) Kinetic study of the oxidation of uranium dioxide. J. Chem. Phys. 27, 137-144

P. Baudoin et al. “Spent fuel performance assessment –SPA project” European Commission, EUR 19132 EN, 2000

J. Bruno, E. Cera, J. de Pablo, L. Duro, S. Jordana, D. Savage, “Determination of radionuclide solubility limits to be used in SR 97. Uncertainties associated to calculated solubilities”, SKB TR 97-33, Svensk Kärnbränslehantering AB (1997)

H. Christensen, Studsvik Report M-97/121, 1997

CNE, Commission nationale d’évaluation, Rapport No. 4, Paris (1998)

Diaz Arocas P., García Serrano J, Mendez F.J., Quiñones J., Rodriguez Almazan J.L., Serrano Agejas J. and Esteban Hernández J.A. (1997). Almacenamiento Definitivo de Residuos de Radiactividad Alta. Pub. Tec. ENRESA 04/97

B. Einziger and R.V.Strain, “Behavior of breached pressurized water reactor spent fuel rods in an air atmosphere between 250 and 360°C”, Nuclear Technology 75 (1986) 82-95

T. Eriksen, “Radiolysis of water within a ruptured fuel element” SKB PR U 96-29 (1996)

B. Finch et al, Spent fuel workshop, Canada (1999)

R. Forsyth, Spent nuclear fuel. A review of properties of possible relevance to corrosion processes. SKB-TR--95-23 (1995)

J. Gimenez, E. Baraj, M. E. Torrero, J. Casas de Pablo Effect of H_2O_2, NaClO and Fe on the dissolution of unirradited UO_2, in NaCl 5 mol kg-1. Comparison with spent fuel dissolution experiments. J. Nucl. Mater. 238, 64-69 (1996).

J.Giménez, M. Molera, I.Casas, M.E. Torrero, J. de Pablo, "Kinetics of reduction and precipitation of U(VI) in the dissolution of UO2 under anoxic conditions in 5 m NaCl

solutions. Influence of metallic iron., Mat. Res. Soc. Symp. Proc. 506, p. 105-122 (1998)

Grambow B., Loida A., Dressler P., Geckeis H., Müller N., Gago J., Casas I., de Pablo J., Giménez J. and Torrero M.E. (1997) Chemistry of the reaction of fabricated and high burnup UO2 fuel with saline brines. Final Report EUR 17111 FI2W-CT90-0055, European Commission.

B. Grambow, A. Loida, A. Martinez-Esparza, P. Diaz-Arocas, J. de Pablo, J.L. Paul, G. Marx, J.P. Glatz, K. Lemmens, K. Ollila, H. Christensen, Source term for performance of assessment of spent fuel as a waste form, European commission, EUR 19140 (2000)

B. Grambow, E. Smailos, H. Geckeis, R. Müller, H. Hentschel, Radiochimica Acta 74, 149-154 (1996)

Grandstaff D.E. (1976) A kinetic study of the dissolution of uraninite. Economic Geology 8, 1493-1506

Gray W.J., Leider H.R. and Steward S.A. (1992) Parametric study of LWR spent fuel dissolution kinetics. J. Nucl. Mat. 190, 46-52.

W.J. Gray, “Spent fuel dissolution rates as a function of burnup and water chemistry”; PNNL-11895, Pacific Northwest National Laboratory, Richland, WA, USA (1998)

W.J. Gray and C.N. Wilson, “Spent Fuel Dissolution Studies. FY 1991 to 1994”, PNL-10540, Pacific Northwest Laboratory (1995)

Guenther, Characterization of spent fuel approved testing material ATM 104”, PNL 5109-104, 1991

B.D. Hanson, “The Burnup Dependence of Light Water Reactor Spent Fuel Oxidation”, PNNL-11929 (1998)

W.Hauser, calculation with program PRODOSS / Version Hp-Vectra, ha 1989-03, KfK/INE (1994)

O.W.Hermann “The Calculation of Se-79 Half-Life from Measured Activities“ Priv.Comm. to ENDSF (1993)

Hiskey J.B.(1979) Kinetics of uranium dioxide dissolution in ammonium carbonate. Trans. Inst. Nin. Metall. Sect. C, 88, C145-C152.

J. Janeczek, R. C. Ewing, Mat. Res. Soc. Symp. Proc. 257, 497-504 (1992)

S.Jiang, J.Guo, S.Jiang, C.Li, A.Cui, M.He, S.Wu, S.Li "Determination of the Half-Life of 79Se with the Accelerator Mass Spectrometry Technique" Nucl.Instrum.Methods Phys.Res. B123, 405 (1997)

J. de Pablo, I. Casas, J. Gimenez, M. Molera, M.E. Torrero, Mat. Res. Soc. Symp. Proc.465.(1997) 535-542.

G.W.Parker, G.E.Creek, G.M.Hebert, P.M.Lantz, W.J.Martin "Radiations and Half-Life of Long-Lived Fission Selenium", ORNL-499, p.45 (1949)

C. Poinssot, J.P. Piron, P. Toulhoat, "Potential internal evolution of spent fuel during 100 –1000 yr prior to access of water in a repository" Spent fuel Workshop, Canada 1999

Posey-Dowty J., Axtmann E., Crerar D., Borcsik M., Ronk A. and Woods W. (1987) Dissolution rate of uraninite and uranium roll-front ores. Economic Geology 82, 184-194.

Shoesmith D.W. and Sunder S., The prediction of nuclear fuel (UO2) dissolution rates under waste disposal conditions (1992). J. Nucl. Mat. 190, 20-35.

SKB, "SR 97 Main report", Technical Report TR99-06, (1999a)

SKB, "SR 97 Processes in the repository evolution" Technical Report TR99-07, (1999b)

SKB, "SR 97, Waste, repository design and sites", Technical Report TR-99-08 (1999c)

SKB, "SR 97, Data and data uncertainties", Technical Report TR-99-09 (1999d)

K. Spahiu et al., Spent fuel Workshop, Canada (1999)

S. Stroes-Gascoyne, Journal of Nuclear Materials 190, 87-100 (1992)

L. E. Thomas, L.A. Charlot, M.H. Engelhard, "Auger analysis of grain boundaries in LWR spent fuel"; quoted in SKB (199b) as "unpublished results of Pacific Northwest Laboratory (1988)

L.E. Thomas, O.D. Slage and R.E. Einziger, "Nonuniform oxidation of LWR spent fuel in air" Journal of Nuclear Materials **184** (1991) 117-126

Thomas G.F and Till G. (1984) The dissolution of unirradiated UO2 fuel pellets under simulated disposal conditions. Nucl. Chem. Waste Manag. 5, 141-147.

Torrero M.E., Baraj E., de Pablo J., Giménez J. and Casas I. (1997) Kinetics of corrosion and dissolution of uranium dioxide as a function of pH. Int. J. Chem. Kinet. 29, 261-267.

Appendix

Evaluation of the SR 97 model for radiolytic fuel dissolution

In SR 97 long-term fuel dissolution rates in groundwater of 10^{-8}/yr are predicted based on radiolysis as the only source of oxidants in an otherwise reducing geochemical environment. A model for radiolytic fuel dissolution is used, based on the work of Eriksen (1996). In this model the concentrations of the radiolysis products H_2O_2 and of O_2 were calculated based on a model for radiolytic decomposition of groundwater, considering simultaneously the consumption of these oxidants by reaction with the fuel surface. The reaction rates of UO_2 with H_2O_2 and O_2 were taken from empirical data of unirradiated UO_2 assuming first order concentration dependency. In the following it will be shown that uncertainties in the calculation of H_2O_2 concentrations are very large, even for deionised water. The empirical relation between H_2O_2 concentrations and UO_2 dissolution rates is not validated with a single experimental data point in the predicted low H_2O_2 concentration range.

Uncertainties in the base model for radiolytic decomposition of water

The base of any model on groundwater radiolysis is the radiolytic reactions in pure water. Rate constants for carbonate or other groundwater ligands are formulated based on these reactions. In order to assess some of the uncertainties, related to the choice in rate constants for radiolytic reactions, the approaches of H. Christensen (Grambow et al. 2000) and of Eriksen (1996) on pure water are compared. A comparison of radiolytic reactions and associated rate constants for deionized water is given in Table A1.

Table A1 : Comparison of rate constants in $dm^3 \cdot mol^{-1} \cdot s^{-1}$ for radiolytic decomposition of deionized water

REACTIONS					Christensen	Eriksen
OH	+H2	=H	+H2O		3.400E+07	4.000E+07
OH	+H2O2	=HO2	+H2O		2.700E+07	
OH	+H2O2	=O2-	+H2O	+H+		2.250E+07
OH	+O2-	=O2	+OH-		1.000E+10	1.000E+10
OH	+HO2	=H2O	+O2		7.100e+09	
OH	+OH	=H2O2			5.550E+09	4.000E+09
OH	+OH-	=H2O	+O-		1.200E+10	

REACTIONS					Christensen	Eriksen
OH	+HO2-	=HO2	+OH-		7.500E+09	
OH	+H	=H2O			7.000E+09	2.50E+10 !
OH	+E-	=OH-			3.100E+10	2.000E+10
OH	+O-	=HO2-			1.800E+10	
O-	+H2O	=OH	+OH-		1.700E+06	
E-	+O2	=O2-			1.900E+10	2.000E+10
E-	+H2O2	=OH	+OH-		1.100E+10	1.600E+10
E-	+O2-	=HO2-	+OH-	-H2O	1.300E+10	1.100E+10
E-	+H+	=H			2.300E+10	2.200E+10
E-	+H2O	=H	+OH-		1.900E+01	2.000E+01
E-	+HO2-	=O-	+OH-		3.500E+09	
E-	+E-	=H2	+OH-	+OH-	5.500E+09	8.000E+09
E-	+HO2	=HO2-			2.000E+10	2.000E+10
E-	+H	=H2	+OH-	-H2O	2.500E+10	2.000E+10
H	+O2	=HO2			2.100E+10	
H	+O2	=O2-	+H+			2.000E+10
H	+O2-	=HO2-			2.000E+10	2.000E+10
H	+H	=H2			7.800E+09	1.000E+10
H	+HO2	=H2O2			2.000E+10	2.000E+10
H	+H2O2	=H2O	+OH		9.000e+07	6.000E+07
H	+OH-	=E-	+H2O		2.200E+07	2.000E+07
HO2	+O2-	=O2	+HO2-		9.600E+07	8.500E+07
HO2	+HO2	=H2O2	+O2		8.400E+05	7.500E+05
HO2		=H+	+O2-		8.000E+05	8.000E+05
H+	+O2-	=HO2			5.000E+10	5.000E+10
H+	+HO2-	=H2O2			2.000E+10	
H2O	+HO2-	=H2O2	+OH-			5.735E+04
H2O2		=H+	+HO2-		3.560E-02	
H2O2	+OH-	=H2O	+HO2-			5.000E+08
H+	+OH-	=H2O			1.430E+11	1.430E+11
H2O		=OH-	+H+		2.599E-05	2.599E-05
O2-	+O2-	=HO2-	+O2	-H+	1.800e+09	*H+
H2O2		= H2O	+O		1.000E-03	*
O	+O	= O2			1.000E+09	*

The comparison shows many similarities in the stoichiometry of reactions and in the rate constants, but there are also differences. In order to find out whether these differences are significant for the final results, calculations were performed with both databases, using G values both for alpha and beta radiation. No G values are reported by

Eriksen (1960), hence G-values of Christensen are used for both calculations as listed in Table A2. The calculations are performed for a dose rate of 685 Gray/h, without considering mass transfer to a gas phase. This dose rate was used in SR 97. Calculations were performed with the computer code Maxima Chemist, the same code was used by Eriksen and by Christensen.

Table A2 : G-values and starting concentrations used for the comparison

	G-values		starting concentrations
	alpha	beta/gamma	mol/kgH2O
H+	0.06E-00	2.76E-00	1.000E-08
OH-		0.10E-00	1.000E-06
H2O	-2.71E-00	-6.87E-00	5.554E+01
H2O2	9.85E-01	7.20E-01	
H2	1.30E-00	0.45E-00	
H	0.21E-00	0.55E-00	
E-	0.06E-00	2.66E-00	
OH	0.24E-00	2.67E-00	
HO2	0.22E-00	0.00E-00	

The calculation results for $1.6 \cdot 10^7$ s are given in Table A3 for alpha and beta/gamma radiolysis. The results of the two databases are quite different. In the case of alpha radiation, high dissolved H_2 concentrations are achieved corresponding to gas pressures of about 1000 bars. In reality, due to mass transfer by diffusion, these concentrations cannot be achieved, not even with the high dose rates close to the fuel surface.

Table A3 : Comparison of the resulting concentrations (mol/kgH_2O) of radiolytic species based on alpha and beta/gamma radiolysis calculations using the databases of either Eriksen (1996) or of Christensen (in Grambow et al. 2000) ($1.6 \cdot 10^7$ s, 685 Gy/h, water, const. pH 8, no HCO_3, absence of gas phase, no UO_2 present)

alpha

	H2O2	HO2-	O2	H2	H	E-	OH
Eriksen	3.5E-01	5.5E-05	2.8E-03	3.5E-01	1.3E-16	2.3E-19	4.2E-16
Christ.	2.9E-05	2.3E-10	1.8E-01	3.6E-01	2.5E-18	3.7E-19	4.2E-16

beta/gamma

	H2O2	HO2-	O2	H2	H	E-	OH
Eriksen	1.1E-07	1.7E-11	9.1E-09	1.2E-07	1.6E-10	1.8E-11	2.1E-09
Christ.	1.6E-07	5.6E-12	1.4E-07	4.4E-07	1.1E-11	9.9E-12	6.5E-10

Therefore, the calculations were repeated assuming presence of a gas phase of equal volume (Table A4).

The results in presence of a gas phase where again quite different for the two databases. Calculated radiolysis gas pressures were similar in the case of alpha irradiation, but in case of beta/gamma radiation, calculated gas pressures were more than an order of magnitude lower for the database of Eriksen (1996).

Table A4 : Comparison of the resulting concentrations (mol/kgH_2O) of radiolytic species in presence of a gas phase based on alpha and beta/gamma radiolysis calculations using the databases of either Eriksen (1996) or of Christensen (in Grambow et al. 2000) (1.6×10^7 s, 685 Gy/h, water, const. pH 8, no HCO_3, volume of gas phase = volume of water, assumption of validity of Henrys law, no UO_2 present)

alpha, with gas phase

(Eriksen: 9.7bar H_2(g), 1.8bar O_2(g)Christensen: 8.1bar H_2(g), 4.0bar O_2(g))

	H2O2	HO2-	O2	H2	H	E-	OH
Eriksen	2.8E-01	4.4E-05	2.3E-03	8.2E-03	1.2E-16	2.8E-19	1.3E-15
Christ.	2.9E-05	5.4E-09	5.4E-03	6.9E-03	8.5E-17	1.2E-17	2.2E-14

beta/gamma, with gas phase

Eriksen 0.001bar H_2(g), 0.0005bar O_2(g) Christ. 0.016 bar H_2(g), 0.008bar O_2

	H2O2	HO2-	O2	H2	H	E-	OH
Eriksen	3.7E-07	5.9E-11	7.1E-07	9.2E-07	3.2E-12	2.6E-12	2.6E-10
Christ.	5.4E-06	9.8E-10	1.1E-05	1.4E-05	9.5E-14	1.0E-11	2.1E-11

Effect of water radiolysis model on fuel dissolution rates

In order to study the effect of the different radiolysis models of deionized water on predicted fuel dissolution rates, the fuel dissolution model of Eriksen (use of calculated radiolytically generated H_2O_2 and O_2 concentrations in empirical UO_2 dissolution rate laws) was used both with the radiolysis model of Eriksen and with the radiolysis model of Christensen. These two models are compared both for alpha and for beta/gamma radiation enhanced fuel dissolution. Comparison is also made with the Christensen

model for fuel dissolution (only combined with the model of Christensen for the radiolytic decomposition of deionized water). The Christensen model is used for the same irradiation conditions as is the Eriksen model: same G-values, same space region of 100 µm, same fuel surface area. The full model of Christensen is more complicated as it involves diffusion of molecular radiolytic species from a 40 µm space region close to the fuel to the bulk water volume. This is not considered in the Eriksen model and was not used in the comparison. The calculations were based on the published information. The results are given in Figure A1 in terms of fractional fuel dissolution rates as a function of time.

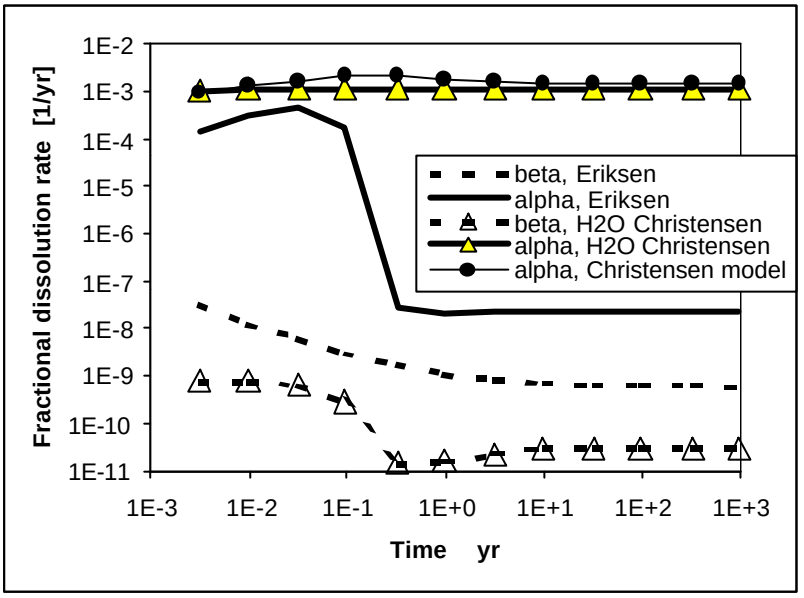

Figure A1: Comparison of the effect of radiolysis models of deionized water on the rate of fuel dissolution

The results show that there are only small differences in the fuel dissolution rates if the same model for the radiolysis of deionized water is used, but there are large differences if different radiolysis models for deionized water are used. These differences are particularly important for long-term alpha radiolysis. The model of Eriksen predicts a decrease in the rates with time by more than 4 orders of magnitude, which is not the case for the Christensen model.

Analyses of radiolysis schemes

In order to analyze as well as to illustrate the reasons for the differences in the corrosion rates for the two models, the radiolytic reaction rate schemes of the two authors are calculated with Maksima Chemist for the case of alpha radiation and in the case of the Christensen model also for beta irradiation. The purpose of this calculations is not to provide a realistic view of the effect of radiation on fuel dissolution, but to show how complicated these reactions are and how much uncertainties are associated to them. The uncertainties cannot be assessed in absolute terms, but it becomes clear from the comparison that the model uncertainty is extremely large.

Transformation rates of individual radiolytic species with respect to other species are calculated from the output of Maksima. The results are given in graphical form in the following Figures A2-5, with the thickness of reaction arrows representing relative reaction rates. Rates of local thermodynamic equilibrium reactions are much faster and are illustrated by two directional arrows. Only the major rate contributions are indicated.

In the model of Christensen, UO_2 dissolution appears to continue under the influence of a constant alpha irradiation dose without significant reduction in reaction rates during 1000 yrs and more. The rate is controlled to about 25% by direct reaction with H_2O_2 and to 75% by the radicals HO_2 and O_2^- both of which are formed to a large extent by radiolytic or non-radiolytic decomposition of H_2O_2. Oxidation by dissolved O_2 is almost negligible. Almost 90% of the produced radiolytic oxidants react with the fuel, indicating that only 10% recombine with reductants (e-, H_2, H) to form water molecules.

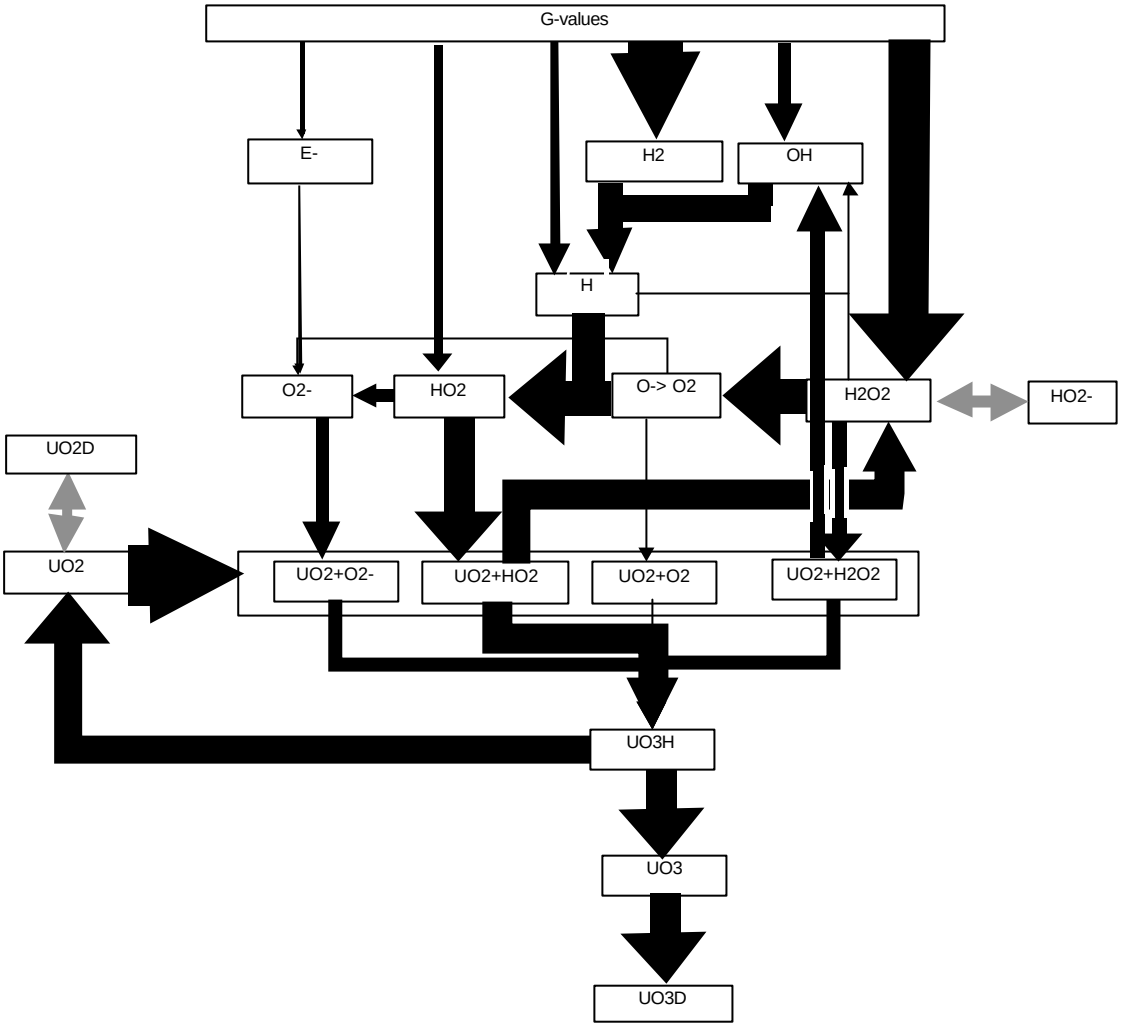

Figure A2: Model by H. Christensen for α radiolytic dissolution of UO2 (UO3H has the average formal U valence of 5, "UO3" represents oxidized UO2, "UO3D" is dissolved fuel, which is removed from the reaction system), calculation without individual gas phase for 1000 yr at 685 Gy/h (the alpha radiation doses at time of disposal in 100 µm water film) at pH 8 in pure water

The situation is different for β radiation in the Christensen model as can be seen from Figure A3a and b excluding and considering diffusion processes. Here, in the case of absence of diffusion the accumulation of H_2 leads to a slow down of reaction rates. Whereas in the case of diffusion, the higher mobility of H_2 with respect to radiolytic oxidants leads to an increase in the local concentration of oxidants close to the fuel surface and in much faster reaction rates. In contrast to the situation with alpha irradiation, the main oxidant in the case of beta irradiation is considered to be the OH radical, whereas H_2O_2 appears to be insignificant. In the presence of H_2, a large quantity of the OH radical is consumed by formation of H radicals. This is not the case, if H_2 is diffusing away.

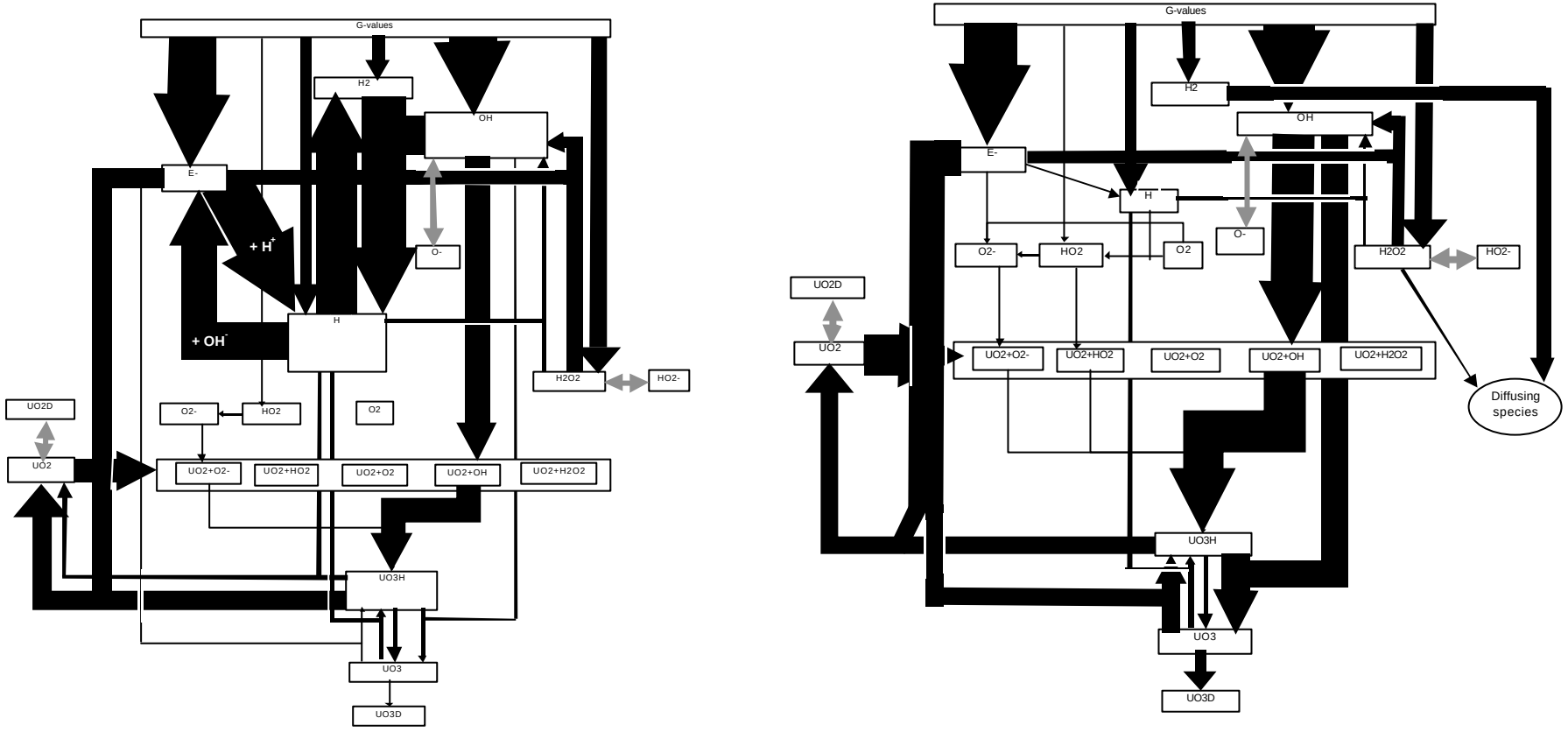

*Figure A3 Model by H. Christensen for **b** radiolytic dissolution of UO2 (UO3H has the average formal U valence of 5, "UO3" represents oxidized UO2, "UO3D" is dissolved fuel, which is removed from the reaction system), calculation without individual gas phase for 10 yr at 685 Gy/h (the **b** radiation doses at time of disposal in 40 µm water film) at pH 7.5 in pure water. Figure A3a: diffusion of molecular radiolytic species is ignored, leading to accumulation of H_2, in Figure A3b the effect of diffusion is considered*

For the model of Eriksen, two calculations are given both only considering alpha irradiation. One calculation is done for 10 d, the other for 1000 yr. In this model the recombination of oxidative and reductive radiolytic species is much more important, even after 10 d.

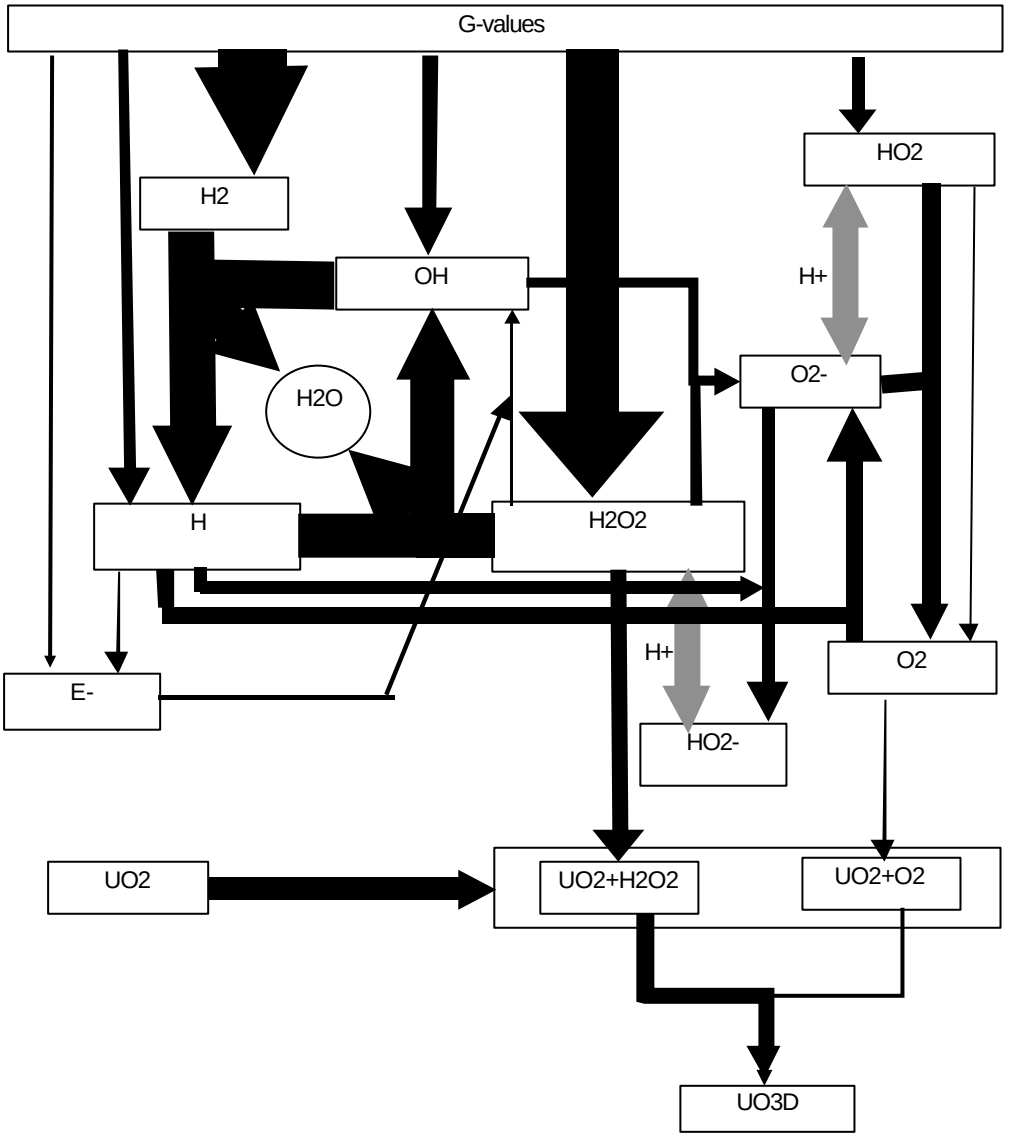

*Figure A4: Model by Eriksen for alpha radiolytic dissolution of UO2 ("UO3D" is dissolved fuel, which is removed from the reaction system), calculation without individual gas phase for **10 d** at 685 Gy/h (the alpha radiation doses at time of disposal in 100 µm water film) at pH 7 in pure water*

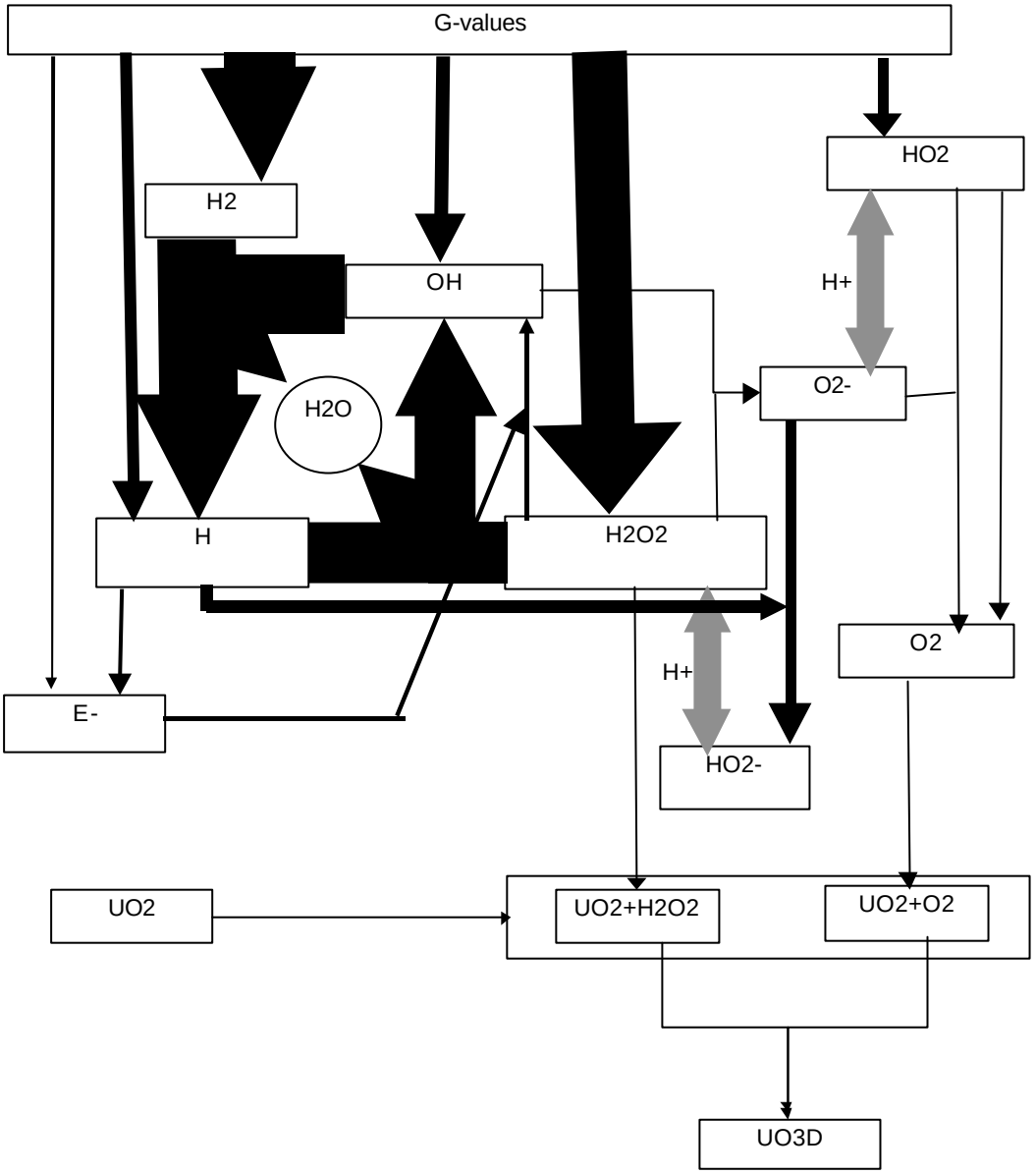

*Figure A5: Model by Eriksen for alpha radiolytic dissolution of UO_2 ("UO3D" is dissolved fuel, which is removed from the reaction system), calculation without individual gas phase for **1000 yr** at 685 Gy/h (the alpha radiation doses at time of disposal in 100 µm water film) at pH 7 in pure water.*

Initial reaction rates are about a factor of 2 lower than in the model of Christensen for pure alpha radiation. After already 30 d this reaction rate decreases by about a factor of 10000, about 20000 times lower than the long-term corrosion rates calculated by the model of Christensen. This decrease is not associated to the enhanced recombination due to increasing dissolved H_2 concentrations with time, because long-term H_2

concentrations are higher in the Christensen model than those in the Eriksen model. Instead, recombination due to H radicals appears to be dominant. 100000 times higher H radical concentrations are achieved in the long-term in the Eriksen model when compared to the Christensen model, though initial H radical concentrations were similar. As a consequence the formation of OH radicals and water molecules by reaction of H radicals with H_2O_2 is much more important in the Eriksen model than in the Christensen model (the corresponding rate constants are similar in the two models, Table A1).

What is the reason for the much lower H radical concentrations in the Christensen model for alpha radiolysis enhanced fuel dissolution? When comparing Figure A2 with Figure A3 and A4 it becomes obvious, that the decomposition of H_2O_2 into O radicals and their recombination product O_2 is the cause. This reaction occurs also in the absence of irradiation. This reaction was suggested by Shoesmith to simulate the catalytic decomposition of H_2O_2 on the surface of UO_2 (Christensen, personal communication). This reaction is not considered in the Eriksen model. It can be see from a comparison of Figures A1 and A2 with Figure A5 that O_2 is considered in the two models as a strong scavenger for H radicals. The more O_2 is generated, the more H radicals are consumed. Long-term O_2 concentrations are about 10 orders of magnitude lower in the Eriksen model when compared to the long-term Christensen model.

In order to test the effect of H_2O_2 auto-decomposition into O_2 for the Eriksen model, respective rate constants of the model of Christensen were introduced into his model. Using this equations, calculated 1000 yr H_2O_2 concentrations became similar in the two models ($3.6 \cdot 10^{-5}$ M for the Christensen model vs. $3.0 \cdot 10^{-5}$ M for the modified Eriksen model) and the corresponding dissolved O_2 concentrations were only a factor of 4 lower in the modified Eriksen model than those of Christensen ($2.0 \cdot 10^{-5}$ vs $5 \cdot 10^{-5}$). Calculated alpha radiolysis enhanced fuel dissolution rates were only about 20% lower in the modified Eriksen model than for Christensen. As in the model of Christensen for alpha radiolysis, no decrease in reaction rates with time was predicted by the modified Eriksen model. However, in contrast to the Christensen model, the dominant fuel dissolution rate became the interaction of the fuel with dissolved O_2.

Conclusions on the use of the radiolysis model of Eriksen in SR 97 performance assessment

One may conclude that large model uncertainties exist in the models for radiolytic fuel dissolution. The major difference in the model of Eriksen and the one of Christensen for alpha radiolysis effects on fuel dissolution, is not the inclusion or exclusion of reactions of radicals with UO_2 (this difference may account for only a variation of a factor of 4 in reaction rates). In contrast the large difference of more than 4 orders of magnitude and the calculated decrease of reaction rates is associated to different reaction schemes for H_2O_2. Large uncertainties still exist in radiolysis models, even for deionized water. ***It appears that the models are not yet validated for long-term reactions. It cannot be recommended to use these models neither for quantitative long-term fuel***

***performance predictions, nor as a qualitative performance indicator*. It can be concluded that the predicted long term corrosion rate of 10^{-8}/yr has not only no experimental base, it also has no reliable theoretical justification.**

Review of SKB's Report, SR 97 – Post-closure Safety

Per Holmlund
Department of Physical Geography
Stockholm University
S-106 91 Stockholm, Sweden

September 5, 2000

Summary
I have read and reviewed the quality and credibility of SKB's SR 97 report, from the perspective of my own expertise.

The climate and glaciation scenarios are described in detail and largely adequately supported by data. The deficiencies that I have chosen to point out are serious from the point of view of principle. I have not attempted to assess the significance of these deficiencies for a future repository.

The climate predictions used in the reports are internationally generally accepted models, which can be said to be uncontroversial. However, they have been overutilized in that too much confidence has been placed in the results. The uncontroversial part of the climate scenario is the predicted development, that is, that there will be alternating cold and warm periods over the next hundred thousand year period, like we have experienced during the last glacial cycle. However, time and temperature data are naturally highly uncertain. As a reviewer, it is difficult for me to understand why priority has not been given to reconstructing events that have occurred at the possible repository sites studied in the report instead of performing general calculations based on the highly inaccurate future scenarios. High resolution data are available from the last glacial cycle. Geological evidence is also available which provides information on temperature conditions within and beneath the ice and, thereby, also provides information on the hydrology of the ice and beneath the ice. We know a great deal about these conditions, but nothing about the future.

The modelling of extent of the ice sheet is not significantly different from other model experiments, which means that it largely reflects what most researchers consider to have occurred and likely to occur. However, the modelling results relating to the temperature distribution are highly controversial. These results are not supported by other modelling data, which on the contrary clearly indicate temperature patterns in and beneath the ice, which deviate from SR 97. The classification into ice divide zones and melting zones lacks a physical basis for the meanings given to these concepts in the report. Although these are only qualitative descriptions of the model designers' assumptions, the results are used quantitatively. Furthermore, the coupling to hydrology includes irrelevant descriptions of how the subglacial drainage in temperate glaciers has a seasonal variation, due to a hydraulic coupling between the surface and the base of the ice. The ice sheets that have covered and will cover Scandinavia are of a cold polar type, which lacks this hydrological coupling between the ice surface and the base, apart from possibly in frontal zones. The report clearly describes the ice as temperate, which must be considered to be an error that has a considerable impact on predictions concerning the subglacial water flow.

GCM models have not been applied. The climate is complex and changes in the topography in the form of a growing North American continental ice sheet, change the circulation pattern and, thereby, the distribution of precipitation. Knowledge is available in this area, but this knowledge is not applied in the report. Furthermore, the fact that no sensitivity tests have been conducted of the climate and glacial scenario is surprising.

The Report

I have reviewed the sections concerning ice modelling, climate and hydrological phenomena in the following reports:

1. *Impact of Long-term Climate Change on Deep Geological Repository for Spent Nuclear Fuel.* (Main text plus Appendices) by Boulton, Kautsky, Morén and Wallroth.
2. *Analysis of Groundwater Flow beneath Ice Sheets* by Boulton, Zatsepin and Maillot.
3. *Climate and Shoreline in Sweden during the Weichsel and the Next 150 000 Years* by Morén and Påsse
4. *Future Glaciation in Fennoscandia*, by Lars Forsström, Posiva 99-30, University of Oulu
5. *Deep Repository for Spent Nuclear Fuel. SR 97: Post-closure Safety.* Background Reports, Main Report Volumes I and II and Main Report with Summary.

General Comments on Scenario Development

The reports are based on a climate scenario, which is based on insolation conditions as well as on ice modelling which describes the extent of the ice sheet, ice thickness and temperature conditions. With respect to the paleoclimatological scenario, it is based on $\delta^{18}O$ analyses from mosses in France as well as on deep-sea cores. The authors have not used ice cores from Greenland, which is surprising. These cores are generally considered to have the highest resolution and to be the most thoroughly measured climate series that are available for the northern hemisphere. However these climate series only date as far back as the past 200,000 years and this is probably why the authors avoided using them. Nevertheless, the authors could have used them in the ice modelling. The important thing is that these data cover more than one glacial cycle.

The scenario for the predictions is based on astronomical factors, such as variations in the Earth's orbit, the angle of the axis of the Earth and its wobbling as well as a prediction for variations in solar activity. The climate prediction is a hundred thousand-year scenario which is in many respects similar to the past one, which can be viewed as a reasonable result. The translation of the astronomic variations into temperature data at the Earth's surface has been done using regression analysis with proxy data for temperature over the past hundred thousand years.

Processes and Initial Conditions

<u>Climate</u>
The work is based on predictions of the future climate based on the astronomic variations in the Earth's orbit around the sun, which results in a varying insolation to the Earth's surface. By studying how the insolation should have varied over the past 100,000 years and by calibrating these oscillations against proxy data for temperatures, we can obtain quite a good idea of the temperatures during the last glacial period. However, it must constantly be taken into account that these are proxy data and not real temperature data. Based on the ice drill cores from Greenland, for example, we can say that the average annual temperature was 10-20 degrees colder than today, during the maximum phase of the last glacial period. A more exact determination of the temperature is not possible. This uncertainty is slightly less important to the modelling of the Weichsel glaciation, since we can also utilize geological data to calibrate our models.

According to the forecast, the insolation conditions over the next 100,000-year period, will be fairly similar to past ones. We can, with great conviction, state that we will have a glaciation which, in its final phase, will correspond to the extent of the Weichsel glaciation. However, modelling ground temperatures and ice sheets based on a guessed climate scenario is a dubious approach. The overall characteristics will be captured, but there will be an enormous margin for error with respect to the details.

Whether or not a glacial period corresponds to a climate that is 10 or 20 degrees colder than the present climate has a considerable impact on the extent of the permafrost, for example. Permafrost has occurred in large parts of Sweden during the last glacial period, which can be seen through preserved sensitive landscape forms as well as through fossil ice wedges in the ground. Permafrost also currently exists in northern Norrland and in the mountains and has a considerable impact on the hydrological cycle, since it closes off aquifers. Near to the Tarfala research station, the depth of the frost is currently about 200 m.

Another problem which is difficult to tackle and which is not dealt with in the report is the impact of the ice sheets on the climate. Morén and Påsse (3) state, on page 16, that they assume that three large ice sheets will occur, over North America, Greenland and Scandinavia. On the other hand, they do not write that the North American ice sheet will affect the climate in Scandinavia since the flow patterns of the atmosphere within the West Wind Drift will be displaced. This can have a dramatic impact on the wind direction and, thereby, on the precipitation pattern over Scandinavia. In the same way, a Scandinavian ice sheet will affect an continental ice sheet over Siberia. However, this is not taken up in the reports. In order to correctly understand how ice over Scandinavia will develop, climate-coupled global models should be used, where flow patterns can be simulated, GCM models.

A wiser and more certain approach to the climate scenario for the future would be to study possible deviations from the past glacial period and to take these into account when determining the details of what happened in the past. The advantage of studying what happened in the past is that, in addition to the uncertain temperature proxy data that exist, there are geological traces, which provide further indications of what actually happened. Calculations of possible future scenarios are interesting but lack credibility when they must be transformed into reality. One compromise would have been to have a retrospective scenario in parallel with the future scenario. With or without such a supplementary scenario, sensitivity tests must be conducted and reported. It is simple to add a description of what would happen, for example, if there was permafrost throughout the entire 100,000 year period, or if the area were covered by a cold or warm ice sheet throughout the same period.

Glaciation Model

The ice modelling leaves much to be desired. I have previously expressed my surprise that so much confidence has been placed in a single individual, Jeff Boulton, who is not an authority on ice modelling and who has not taken the effort to fully understand the issue. The modelling results are controversial and have very little support in geological data. The most surprising aspect is the temperature distribution in the ice that is described. The distribution between where the base of a modelled ice sheet, which covers Scandinavia melts and where it is frozen is determined by physics and the climate parameters provided as input data in the model. I have not had an opportunity to

study the structure of the model and to determine which sensitivity tests have been conducted. Nevertheless, the presented temperature distribution is not very probable if a comparison is made with other modelling attempts or with, for example, the current continental ice sheet in Greenland. In accordance with most studies a ”normal” base temperature distribution generally results in basal melting conditions where the ice is thickest and outside this area cold conditions, apart for in a frontal zone (ten or twenty kilometres) where the basal melting occurs again. It is naturally difficult to model exactly where these zones lie. However, it is considerable importance for the calculation of subglacial water flows.

A serious omission is that the author indirectly equates basal melting conditions with the ice being fully temperatre that is permeable to melt water from the surface. This must be considered to be directly incorrect or, at least, highly controversial. Polar ice of the type that has covered, or will cover Scandinavia in the future, is being formed in a climate which is at least 10-15 degrees colder than the present climate and the accumulation area of the ice sheet is within an altitude interval of 1,500-2,000 above seal level. With a normal adiabatic temperature decrease with height, this means that the average annual temperature within the area, if we assume that it is located in the middle of Sweden, is about –25 to -35°C . The ice that is formed will be very cold and this means that it will be impermeable to any meltwater that can be formed at the surface at lower altitudes. The water will not reach the bottom. However, an ice current or offshoots of the continental ice sheet which have moved a long distance or has moved rapidly can, through internal deformation heat, reach the pressure melting point at the base and be temperate at the front zone. One good example of this is the westcoast of Greenland where a boundary zone with a breadth of ten to twenty kilometres comprises ice, which can let through water from the surface. Only here is there a certain seasonal impact on the subglacial water flow. This means that any talk about a seasonal variation in the water flow beneath the ice sheet must be considered to be incorrect as long as the front zone is not taken intended.

The potential impact of water, in a randomly selected site in Sweden, from a future continental ice sheet should be significant when the ice front passes the site. After this, the best guess is frozen conditions. An exception is the southern part of the Gulf of Bothnia where we can expect that the maximum size is to occur as well as the fact that we have an ice flow in the Baltic at the maximum extension. In these areas, it is probable that there will be melt water from the base of the ice as well as glacial erosion. If we move in a westerly direction, there is no reason to believe that basal melting conditions will occur. We can expect deep permafrost there. Therefore, there is a very large difference between Äspö, on the one hand, and the Småland highlands on the other hand. The same applies wherever conditions are studied anywhere along the coast.

In summary, it can be said that the description provided in SR97 of the extent of the ice cover is probably reasonable, its base temperature conditions are controversial (incorrect in my opinion) and the vertical temperature distribution of the ice contains considerable misinterpretations. No connection is shown between Boulton’s model and the temperature results given namely the climate parameters that were applied in this particular calculation.

These views affect the groundwater flow in the potential sites during a glaciation. Adjustments of the calculations, along the lines of what I have suggested, would probably lead to a reduced potential

water flow at a repository site although, on the other hand, it can affect the stresses in the rock during a glaciation.

Detailed Comments

4. Future Glaciation in Fennoscandia

Page 15, third paragraph. The author assumes that the glacial erosion will not exceed 10 m. He does not specify how he has arrived at that figure. If the model applied by SKB of the subglacial temperature conditions during glaciation were correct, which I do not believe to be the case, the erosion during a glacial cycle would be at above 50 m in, for example, the Stockholm area. If negligible erosion is assumed, this would contradict the ice model used.

Page 15, fourth paragraph. The ice is thinner than several models suggest. Furthermore, these low values are not justified.

Page 23, first paragraph. The author says that when an ice sheet advances a permafrost terrain, the ground surface heats up quickly below the ice. In general, this must be viewed as incorrect. This could occur if the ice is warm inside, but this condition does not apply to polar ice.

Page 23, second paragraph. The frozen zone is described as growing as the ice grows. This statement is based only on Boulton's model result, which in turn, is based on his controversial view of the temperature distribution of the ice.

Page 23, second paragraph. The author states that typical runoff values for Quarternary period ice sheets are 0.2 – 0.5 km^3/year. Where do these values come from and on what are they based?

Page 24, third paragraph. Glaciations grind oxidized surfaces and leave clean unweathered surfaces. This occurs in the areas where the base of the ice is at the pressure melting point but does not otherwise occur. If the author had studied the geological literature at the same time that he had studied Boulton's results, he would have detected these contradictions. The continental ice sheet which was once located over Scandinavia was not of the type described by Boulton. Therefore, valid conclusions can not be drawn from it.

5. Deep Repository for Spent Nuclear Fuel. SR97 – Post-closure Safety Volume II

Page 342, Figure 10-2. The diagram that describes the period of 0-150,000 BP does not present the generally accepted perception of how the climate has varied. The period of 110,000-80,000 is called Weichsel I in geology and was colder than the present climate.

Page 354, fourth paragraph. The ground is frozen below the ice divide zone. This is too general a statement which is not supported by calculations and/or modelling work.

Page 355, second paragraph. The content of this paragraph is incorrect. It would be valid if the glacier was of the warm maritime type such as the present-day Vattnajökull, but no one could possibly believe that the Scandinavian ice sheet looked like that. The paragraph shows basic deficiencies in an understanding of physics as well as glaciology.

Page 355, third paragraph. The drainage system is determined by the winter basal meltwater discharges. Apart from below the front zone there is no seasonal variation in the subglacial water flow. Therefore, the text is misleading.

Page 358, Figure 10-14. The diagram is attractive and easy to read, but contains dubious data and controversial results. A corresponding diagram should also have been made for the most recent glaciation. It would result in significantly longer periods of permafrost and frozen basal conditions than shown here. In my opinion, the future scenario is incorrect.

Page 359, the first paragraph under Beberg. The temperature given is –2 to –3 degrees. This illustrates the problems that can arise when too much reliance is placed on models. A more correct value would be 0 to 10 degrees. It would then have been possible to understand the extent of the uncertainty. The results mean that there could easily have been a very deep permafrost during the period.

Page 359, last paragraph. This paragraph states that the ice is in a basal melting zone. This statement is not supported by anything other than a single ice model, i.e. the model used by SKB. It is more probable that the base is frozen.

Page 360, second and eighth paragraph as well as page 361, second paragraph. Once again, the reasoning is based on a single ice model and is highly controversial.

Page 368, third paragraph. Within the area that Boulton specifies to be the melting zone, it is debatable whether or not there should be melting. Different models give different answers. However, the statement that water mass will be added from the surface of the ice during the melting season can be directly rejected as incorrect.

Page 368, last paragraph. The information on retreat rates is not treated critically enough. The melting rate from a collapsed ice sheet in inland Norrland cannot be compared with the change in the retiring ice front of a continental ice sheet with a somewhat functioning mass turnover.

The author

Per Holmlund is professor in Glaciology at Stockholm University. He has a PhD (glacial hydrology and glacial climatology) in Physical Geography and is docent in Glaciology at Stockholm University. In 1996 he was appointed as director for Tarfala Research Station and in 1999 professor in glaciology, with climatic aspects, at Stockholm University. Since the late 1980s he has run the glacio-climatic research programme at Tarfala Research Station and the Swedish glaciological programme in East Antarctica. He has attended 6 major expeditions to the Arctic and Antarctic. In 1991 he began an ice sheet modelling programme financed by SKN/SKI. The first modelling phase was finished in 1995 and a renewed modelling programme is presently carried out in cooperation with SGU. This programme aims at analysing the interaction between ice sheets and the landscape. Per Holmlund is actively working in international panels on glacier mass balance issues in the Arctic and in Antarctica. He represents Sweden in about ten international research committees, and is deeply involved in national developments in polar and geoscientific research issues. Holmlund has published about 80 papers on ice sheet modelling, glacier mass balance and glacier hydrology with relevance to future perspectives on nuclear vaste storage.

Comments Regarding the Bentonite Barrier – SR 97 Post-closure Safety

Göran Sällfors

Department of Geotechnical Engineering
Chalmers University of Technology
S-412 96 Göteborg, Sweden

Summary

This review only deals with the role of the bentonite for ensuring the integrity of the canister from the start and throughout the lifetime of the repository

The following subsections in the reports listed have been studied:

TR-99-06, Sections 4.2, 5.7, 6.1.-6.4., 8.6.-8.7., 11.4.
TR-99-07, Sections 4.12.-4.6.
TR-99-08, Chapter 3
TR-99-09, Sections 5.3.-5.5.
TR-99-32, Full report

Detailed comments and references to specific pages in the reports are given in the enclosed appendix.

It seems as the technical reports in question deliver convincing data and answers to most of the questions that can be raised concerning the bentonite and the interplay between the different processes at hand. However, there is one area where further analysis and discussions seem inevitable. This area is related to the thermo-hydrological behavior of the bentonite, especially during the first phase of the repository. This is discussed in some detail below.

The bentonite is compacted to a high density before installation and has a degree of saturation of about 80 % when it is placed in the bedrock and around the canister. The bentonite is then expected to gradually increase its water content by uptake of water from the surrounding bedrock. Thereby, the bentonite will swell and completely fill the gap between the canister and the bentonite and between the bentonite and the bedrock as well as exert radial pressure on the canister itself. It is well known that the hydraulic conductivity and the heat conductivity of the bentonite to a large extent depend on the degree of saturation. In the reports it is obvious that the pore pressure in the surrounding bedrock is expected to be large, close to 500 kPa. This high pressure, together with the suction in the bentonite, is expected to result in a rather quick saturation of the bentonite around the canister.

The same processes are expected to rather quickly saturate the backfill, consisting of a mixture of crushed bedrock and bentonite in the tunnels above the deposition holes. These processes have been analyzed by means of finite element analysis. The time required is comparatively short and the resulting temperatures in the bentonite close to the canister will be acceptable.

Questions can, however, be raised regarding the boundary conditions assumed for the pressures and the flow capacity of the bedrock. This is important as, if the degree of saturation of the bentonite becomes too low, the temperature of the canister might force a movement of water away from the canister, thus lowering the degree of saturation of the bentonite. Then the thermal conductivity of the bentonite will decrease, and the temperature of the bentonite could start increasing, whereby irreversible processes could occur in the bentonite. This could, in turn, result in a much higher hydraulic conductivity for the bentonite, making the barrier less effective than anticipated.

During the tests in the Stripa project, it was found that there was a possibility of holes being fairly ‘dry’, as very little water came from the bedrock and hardly any cracks crossed the hole. This has been accounted for in the analysis by studying the case where the bentonite is saturated by flow of water from the backfill in the tunnel above. This analysis also assumes 500 kPa pore water pressure at the boundary of the tunnel. If this is the case, then the analysis seems reasonable and the wetting procedure is comparatively rapid. However, this begs the question of how long it will take to restore the pore pressures that existed around the tunnel in the bedrock before the tunnel was excavated? After the tunnel is excavated, it will take some 40 years before the whole site is filled with canisters and the tunnel is closed off. The problem that needs to be given some more attention is how the sequence of using the holes should be planned and how the pore pressures can be expected to be restored to its original values or at least parts of it. If the time delay is too large, there might be a risk of obtaining too high temperatures in the bentonite, which might cause unexpected and unwanted changes in the properties of the bentonite.

Appendix

Comments regarding the bentonite barrier - SR-97, Post Closure Safety

TR-99-07, Processes in the repository evolution.

Sections studied: Chapter 4, Sections 4.1 – 4.6

This chapter is overall well written and principally addresses all the relevant questions within this framework. There is one main question, where the answer is taken for granted without considering the background, i.e. saturation of the buffer material and the backfill material. In most places the text reads ..after saturation….. or …when the buffer material is saturated…However, saturation is not treated as a process in the repository evolution, which I definitely think it should be. It is, though, dealt with in the main report, volume one, and I will comment on this there.

In section 4.5.1 it is stated that "it is not important to know all the details of the saturation process for the safety assessment". Perhaps not, but more so than is indicated in this report.

It is important to note the results from the Stripa tests with regards to the degree of saturation. Great variations were observed. In this report (p 106) near water saturation is interpreted for samples showing 80 % of saturation. This is not in line with common practice.

When discussing the time perspective, it is stated that "counting starts, that is 10-15 years" (p 107) but not when it is started, i.e. after placing the canister, after closure of the individual hole, after closing a section of the repository or after the complete repository is closed.

In section 4.6, where most relevant problems are discussed, it is correctly stated that "…need to be done to improve our understanding .." (p 119), referring to the unsaturated stage.

Finally a few minor comments:

Page 98m. "At application, the water saturation of the blocks is lower, but their dry density is higher, which gives approximately the same thermal conductivity." The swelling will not be at all so high as to compensate for the increased conductivity due to the increasing degree of saturation.

Page 100m. A number of factors affecting the temperature are given, but the most important, the buffer material and its properties, depending on degree of saturation, is left out.

Page 103u. Why is A2 left out?

Page 105m. High salinity may be good for the saturation process, but the whole purpose of the buffer material is to constitute a barrier with extremely low hydraulic conductivity.

TR – 99 –08, Waste, repository design and sites.

Sections studied: Chapter 3.

This report is rather descriptive, but still contains some contradictory statements. It is, for example, stated on p 24u, "…bentonite blocks, pressed to a high degree of water saturation…" This is not quite in line with procedures described elsewhere. Nor is the statement later in the same paragraph "…so that a high pore water pressure in the bentonite is reached quickly". This gives the impression that the high pore water pressures will develop long before the repository is closed, which is not the case. In the following section on the backfill, there is no mention of the saturation of the backfill.

TR – 99 – 09, Data and data uncertainties

Sections studied: Sections 5.3.-5.4.

No critical comments, except for perhaps a warning that the De is very difficult to determine and might vary quite a lot.

TR – 99 –32, Creep in buffer clay (Roland Pusch)

Section studied: Full report

Well written, reasonable results.

TR – 99 –06, Main Report, Volume I

Sections studied: 4.2., 5.7., 6.1-6.4, 8.6-8.7

In general, it should be stated that the report gives an impression of being well well worked out and very well written. It is comprehensive and seems to cover all essential parts of the full process.

In section 4.2. the system for illustrating the different processes and the links between them is indeed clear and well focused. This seems also to be the case for section 5.7., where no critical comments can be made.

Also sections 6.1. – 6.4. are reasonable and well backed up by references. However, most discussions are made under the assumption that the buffer material quickly gets saturated and that the pressure in the water in the bedrock is almost unaffected by the excavation. This is dealt with later in sections 8.6.1. – 8.6.2. Given the assumptions made, the conclusions seem correct. Some of these assumptions, however, need further validation. This will be further commented on in sections 8.6.1. – 8.6.2.

In section 8.6.2. it is noted that credit can not be taken for the water saturation in the buffer material when it comes to maximum temperature in the canister (page 147 bottom). And on page 153 it is stated 'The detailed sequence of events in the saturation process is not important to describe in the safety assessment. That may well be so, but the consequence for the development of the temperature in the buffer material adjacent to the canister is important, as too high temperatures may lead to irreversible processes in the bentonite. I think that on top of page 154 another point should be added dealing with the process of saturation. This becomes especially important for a 'dry' hole, where saturation has to be accomplished through flow through the backfill, see also page 165, last paragraph. In section 8.7.5 it is stated that the process of saturation through the backfill has not been modelled.

A threat to the buffer material is definitely too high temperatures, which possibly could develop if the buffer has a fairly low degree of saturation. This figure is, upon installation, assumed to be 80% of saturation. This number might decrease in a 'dry' hole if the temperature gradients become high. I do not think that they have paid enough attention to the question of saturation of the buffer material through the backfill. Important boundary conditions are then the water pressure in the nearfield of the bedrock, as the backfill material does not at all have the same 'suction potential' as the buffer and will thus probably saturate at a much slower rate.

TR – 99 –06, Main Report, Volume II

Sections studied: 11.4.

no objections

The autor

Göran B Sällfors, born 9th of March 1946

Degrees

Master of Civil Engineering, Lunds Tekniska Högskola, 1971
Doctor of Science, Geotechnical Department, Chalmers Univ. of Technology, 1975
Docent, Geotechnical Department, Chalmers University of Technology, 1980

EMPLOYMENT, PROFESSIONAL EXPERIENCE

Research assistant, Geotechnical Department, CTH 1971-1975
Associate Professor, Geotechnical Department, CTH 1975-1990
Professor, Geotechnical Department, CTH 1991 -
Associate Professor, at Duke University, 1982-1983
Visiting Professor at Duke University, (2 months/year), 1984, 1985 and 1986
Visiting Professor at Purdue University, 1990 (6 months)
Visiting Professor at Norh Carolina State University, 1993 (5 months)
Private consultant 1975-

Member of numerous national and international Committees
Have participated in many European and International Conferences and as key speaker, state-of-the-art reporter at close to 10 conferences

Review of Sorption and Diffusion Data for SR 97

Mike Stenhouse

Monitor Scientific, LLC
3900 S. Wadsworth Blvd., Suite 555
Denver, Colorado 80235, USA

Summary

The approach of SKB in providing K_d values for transport calculations for SR 97, as described in Carbol and Engkvist (1997), and adopted by Andersson (1999), has been to provide what is termed a *reasonable estimate* for the sorption of each radioelement on granitic rock under saline and non-saline groundwater conditions, as well as a corresponding *uncertainty range* based on available experimental data.

Typical treatments of input data for K_d values in the past have been to provide "realistic" and "conservative" estimates of K_d values, but the precise meaning of "conservative" has often been vague and inconsistent. Thus, the approach by Carbol and Engkvist (1997), to provide a *reasonable estimate* supported by an uncertainty range for saline and non-saline conditions, is a different but reasonable methodology for the treatment of K_d values.

Carbol and Engkvist (1997) have updated the review of sorption data and associated recommendations by Albinsson (1991), provided for the SKB 91 safety assessment. The update consisted of an examination of additional experimental sorption data published since the initial review in 1991, with modification of the recommendations of Albinsson (1991) where warranted. The new data are not presented, although references are provided.

Bruno and Duro (1997) reviewed the recommendations of Carbol and Engkvist (1997), and were able to provide additional experimental data from the literature, although no experimental details were provided concerning new sorption data cited. Based on their review, Bruno and Duro (1997) made some reasonable recommendations.. Although not taken into account in the database in Andersson (1999), the effect of such recommendations, particularly for Sr, will be covered by uncertainty range calculations.

Given the importance of K_d as a retardation parameter, the uncertainty ranges appear relatively narrow. There is a danger that the ranges will be treated as absolute, when frequently they are based generally on a small number of experimental data or even a lack of experimental data for the rock water systems being studied.

There is always likely to be a lack of experimental data to support what is effectively expert judgement. Therefore, the best management approach is to focus on those elements for which no data exist (to confirm or update current recommendations, as appropriate), or for radionuclides which appear as key contributors to dose. In the latter case, variation in K_d values can be explored by sensitivity analysis and, where a factor of 10 reduction is significant in terms of a radionuclide's contribution to total dose, experimental work should be carried out. Thus, Andersson's recommendation for probabilistic cases should ensure that any K_d-limiting cases are identified.

Radionuclide transport through the bentonite buffer is taken into account via diffusion, with sorption where merited. The input parameters required, therefore, are effective diffusion coefficient, D_e, distribution coefficient, K_d, and porosity, e. Andersson (1999) notes that the code used by SKB to model migration through the near field can use only one value of porosity, which leads to logistical problems regarding data input. In particular, K_d values must be 'manipulated' to yield a D_e (effective diffusion coefficient) value representative of the transport porosity and the true sorption capacity for that

radionuclide. In this regard, comparison of K_d values with other programmes must be treated with caution.

For input to the work of Yu and Neretnieks (1997), who provided recommendations on relevant K_d values for sorption on compacted bentonite, the lack of a reference porewater seems a major omission. The omission may well have been influenced by the lack of a consensus in how to establish a reference porewater composition.

It is now well established that K_d values obtained from batch sorption experiments must be treated with caution when applying such values to sorption on compacted bentonite. In particular, measurements using disaggregated bentonite samples effectively ignore the partially mobile fraction. Consequently, the erroneously high (non-conservative) batch K_d values result in calculated values for D_e, for bulk intact bentonite which are, in turn, too high.

In terms of experimental work on sorption of radioelements on compacted bentonite, the need for a database of well-documented diffusion (apparent and intrinsic) and sorption data was recognized at a recent Workshop (Huigi and Apted, 1998). Ideally, effective (intrinsic) and apparent diffusion coefficients should be carried out on the same compacted bentonite sample. Any variation of this approach should be interpreted with caution.

The topic of surface diffusion in compacted bentonite continues to generate heated debate, which has still not been resolved by recent experimental or theoretical methods. In this context, the comment by Ochs (1997), that K_d values cannot and should not be evaluated independently of the diffusion model used (*i.e.* with or without surface diffusion), is an important statement. Given that the near-field release code COMP23 applies a traditional diffusion model, the data input should be consistent with this model.

In justifying the selection of K_d value recommendations, Andersson (1999) makes a series of assumptions and arguments which are clearly stated and sensible. He takes account of all the relevant comments from the review of Ochs (1997) as well as the modelling calculations performed by Bruno et al. (1999) on bentonite-groundwater interactions and bentonite porewater evolution.

1.0 Sorption of Radioelements on Granitic Rock

The following references were reviewed in detail:

- *Section 5.6,* Andersson (1999);
- Carbol and Engkvist (1997);
- Bruno and Duro (1997).

In addition to the above, other references quoted in the bibliography were consulted as discussed in the text.

1.1 General Review Comments

The starting point for this review was the report by Andersson (1999) which discusses uncertainties in data input for performance assessment, including sorption and diffusion data.

Carbol and Engkvist (1997) chose to update the recommendations of Albinsson (1991) for SKB 91 based on new experimental data compiled since 1991. These authors note that there is a limited number of sources for relevant sorption data, which is true. Thus, detailed statistical treatment of raw data is generally not possible. The statement by Bruno and Duro (1997) is particularly true:

> "*The nature of K_d means that stochastic analysis of the data are not very useful because the variability in the K_d determined by different workers is mainly originated by the different experimental conditions under which the parameter was determined, and not by analytical error.*"

With respect to groundwater composition, key parameters are pH (sorption by surface complexation), *Eh* (radioelements exhibiting redox-sensitive behaviour), ionic strength (sorption by ion exchange), and specific metal complexants such as SO_4^{2-} and HCO_3^- /CO_3^{2-}.

The realistic estimates of Carbol and Engkvist (1997) are generally consistent and supported by good scientific arguments (expected chemical behaviour, analogy to other elements). Recommended ranges are also reasonable for the most part, although sensitivity analysis should be used to explore the importance of the lower limit of each range. There are still substantial gaps in experimental data for radioelement sorption. If, based on the lower limit of an uncertainty range, a radionuclide makes a significant contribution to total dose, or if experimental data are lacking completely, then additional experiments should be carried out using the elements identified.

Andersson (1999) has chosen to accept the recommendations of Carbol and Engkvist (1997) without modification. He notes that Carbol and Engkvist (1997) attach more importance to the groundwater composition than to the nature of the rock minerals, despite the concerns raised by Bruno and Duro (1997) about the importance of the solid phase. Carbol and Engkvist (1997) conclude that almost always the same highly sorbing minerals are present in rock, although in different proportions, whereas Bruno and Duro (1997) highlight the importance of fracture filling minerals which are exposed initially to the radionuclides during groundwater transport.

In reviewing the recommendations of Carbol and Engkvist (1997), Bruno and Duro (1997) were able to provide additional experimental data from the literature. However, no experimental details were provided concerning the new sorption data. In any case, there is the potential for creating a bias when comparing recommended K_d values with only one set, or at most a few sets of experimental data.

The review of Bruno and Duro (1997) led to the following reasonable recommendations:

- decrease the K_d for Sr under saline conditions by a factor of 10;
- differentiate between K_d values for oxidised and reduced forms of Se, with a value of 0 m^3/kg selected for the oxidised form, *cf.* 0.001 m^3/kg for reduced form
- reduce the upper limit of K_d for Pa to 1 m^3/kg;
- reduce the recommended K_d value of Pu to 1 m^3/kg.

Although not taken into account in the database in Andersson (1999), the effect of such values, particularly for Sr, will be covered by uncertainty range calculations.

Based on this additional information, most of the revised K_d values, provided by Carbol and Engkvist (1997) and adopted by Andersson (1999), have not changed significantly (*i.e.* by more than a factor of 2; see *Table 1*). The major exceptions apply to the following elements:

- Sr (K_d value for non-saline groundwater conditions reduced by factor of 5; for saline groundwater conditions by a factor of 50);
- Pd (K_d value increased by factor of 100 for non-saline groundwater conditions, and 10 for saline);

Ra (K_d values for non-saline and saline groundwater conditions reduced by factor of 5).

Interestingly, the increases recommended for Pd (realistic x100 larger) were made although no additional experimental data were cited for this element. Each uncertainty range provided typically spans one order of magnitude, which is often small in comparison with the spread of experimental data. The lower limit in each range varies from a factor of typically 2-5 less than the corresponding reasonable estimate, with the exception of Pd (factors 10 and 100 less). The small difference (factor 2-5) presumably reflects the fact that the reasonable estimate is skewed towards the lower end of each range, which represents a suitably conservative selection for the reasonable estimate.

Given the importance of K_d as a retardation parameter, the uncertainty ranges appear relatively narrow. There is a danger that the ranges will be treated as absolute, when frequently they are based generally on a small number of experimental data or even a lack of experimental data for the rock water systems being studied.

Andersson (1999) notes that the lower end of the uncertainty range quoted would be a "clearly pessimistic selection". However, this lower end is typically a factor of 2-5 less than the realistic value, *cf.* factor of at least 10 in previous sorption databases. Only in the case of Pd, is the uncertainty range a factor of 10-100 less.

Andersson (1999) refers to the uncertainty ranges of Carbol and Engkvist (1997) as "wide", but the ranges rarely span more than 2 orders of magnitude which is not

particularly wide when compared with the typical variability of experimental K_d values. Thus, their statement that this lower limit "would cover both the experimental uncertainties and the uncertainty in water chemistry at the sites" may not be valid.

There is always likely to be a lack of experimental data to support what is effectively expert judgement. Therefore, the best management approach is to focus on those elements for which no data exist (to confirm or update current recommendations, as appropriate), or for radionuclides which appear as key contributors to dose. In the latter case, variation in K_d

TABLE 1: Comparison of Kd values (m^3/kg)

Radio-element	Albinsson (1991) *Realistic*	Carbol and Engkvist (1997) *Reasonable*	Carbol and Engkvist (1997) *Uncertainty Range*	Bruno and Duro (1997) *Reasonable*	Bruno and Duro (1997) *Uncertainty Range*	COMMENT
C	0.001	0.001	0.0005-0.005 ??	agreed	agreed	C&E: 0.002 upper limit quoted in Table 12-1
Cl	0	0	N/A	agreed	agreed	
Co	N/A	0.1 0.02	0.05-0.5 non-saline 0.01-0.1 saline	agreed ? agreed ?	0.01-0.5 both " " "	B&D: recommend one range only
Ni	0.1 non-saline 0.02 saline	0.1 0.02	0.05-0.5 non-saline 0.01-0.1 saline	agreed ? agreed ?	0.01-0.5 both " " "	B&D: recommend one range only
Se	0.001	0.001	0.0005-0.005	0 oxidising 0.001 reducing	N/A 0.0005-0.005	B&D: separate oxidation states
Kr		0	N/A			radionuclide present as gas
Sr	0.05 non-saline 0.01 saline	0.01 non-saline 0.0002 saline	0.005-0.05 non-saline 0.0001-0.001 saline	agreed 0.00002 sal.	agreed 0.00001-0.0001 sal.	B&D: reduction by factor of 10
Zr	2	1	0.5-3	agreed	agreed	new experimental data required
Nb	2	1	0.5-3	agreed	no assessment	new experimental data required
Tc (IV) Tc (VII)	2 N/A	1 0	0.3-3 N/A	agreed >0 ?	agreed 0.01-1.0	B&D recommendation too high
Pd	0.001	0.1 non-saline 0.01 saline	0.01-0.5 0.001-0.05	agreed ?	no assessment	new experimental data required
Ag (= Cs)	---	0.5 non-saline 0.05 saline	0.1-1.0 non-saline 0.01-0.1 saline	no assessment no assessment	agreed agreed	B&D: scarcity of data
Cd	---	0.1 non-saline 0.02 saline	0.05-0.5 non-saline?? 0.01-0.1 saline??	? ?	agreed ? agreed ?	Ni not good analogue > pH 7
Sn	0.001	0.001	0-0.01 ??	agreed	agreed	C&E: range not discussed
I	0	0	N/A	agreed	agreed	
Cs	0.25 non-saline 0.05 saline	0.5 non-saline 0.05 saline	0.1-1.0 non-saline 0.01-0.1 saline	agreed agreed	0.01-1.0 both " " "	B&D: recommend one range only
Pb	1	N/A	N/A			
Ra	0.5 non-saline 0.1 saline	0.1 non-saline 0.02 saline	0.05-0.5 non-saline 0.01-0.1 saline	agreed ? agreed ?	no range no range	B&D: scarcity of data makes uncertainty range impractical
Ac	3	3	1-5			
Th	5	5	1-10	agreed	agreed	
Pa	2	1	0.5-5	agreed	0.5-1.0	B&D: recommend more restricted range
U (IV) U (VI)	5 N/A	5 0.01 non-saline 0.005 saline	1-10 0.005-0.02 non-saline 0.001-0.01 saline	agreed agreed ? agreed ?	agreed 0.001-0.02 both " " "	B&D: carbonate is key variable rather than ionic strength
Np (IV) Np (V)	5 N/A	5 0.01 non-saline 0.005 saline	1-10 0.005-0.05 non-saline 0.001-0.01 saline	agreed ? agreed agreed	agreed ? 0.001-0.05 both " " "	
Pu	3	5	1-10	1	0.1-5	
Am	3	3	1-10 ??	agreed	agreed	C&E: more restricted range in Table 12-1
Cm	3	3	1-10 ??	agreed	agreed	C&E: more restricted range in Table 12-1
Lanthanides	3	2	1-5	agreed	agreed	

N/A = no entry or not applicable.

agreed?: no explicit agreement with realistic estimate or recommended range.

values can be explored by sensitivity analysis and, where a factor of 10 reduction is significant in terms of a radionuclide's contribution to total dose, experimental work should be carried out. Thus, Andersson's recommendation for probabilistic cases should ensure that any K_d-limiting cases are identified.

1.2 Detailed Comments

1.2.1 Treatment of uncertainty

SKB's treatment of uncertainty in the calculations (Andersson 1999) consists of providing a range of values to be explored in terms of sensitivity analysis. Andersson's recommendation for probabilistic cases should ensure that any K_d-limiting cases are identified.

Under certain circumstances, recommendations for K_d values can be supported by both chemical analogues and thermodynamic modeling. Chemical analogues are acceptable as long as there is strong support for identical chemistry between elements. However, where the distribution in metal complexes as a function of pH is seen to vary substantially, analogue behaviour is difficult to justify. This is the case for Ni and Pd as shown by Bruno and Duro (1997) where similar chemical behaviour was apparent at pH < 7, but was shown to vary above pH 7. Thermodynamic modeling is useful as long as there are adequate thermodynamic data to support the calculations. While this is true for certain elements, it is not the case for most.

In the same context, the findings from the Grimsel *in situ* radionuclide migration experiments (Heer and Smith, 1998) supported a dual-porosity model and the K_d values derived from the migration experiments agreed well with batch sorption data.

1.2.2 Experimental Data

The sorption data reviewed by Albinsson (1991) are obviously relevant to the review by Carbol and Engkvist (1997), but these data are not presented either in Carbol and Engkvist (1997) or in Bruno and Duro (1997), making a comprehensive review of sorption recommendations difficult. Similarly, the review of Bruno and Duro (1997) suffers from not providing all references for sorption data or recommendations provided in comparison diagrams. Furthermore, their presentation of K_d values in diagrams is inconsistent; sometimes including national waste programme recommendations, sometimes not.

Andersson (1999) is probably being overly generous when he states that differences in experimental data arise mainly from differences in groundwater composition. Although groundwater composition plays a major role in determining K_d values, many sorption measurements in the past have been performed without due care to identifying and quantifying the key factors that contribute to K_d variability (with the definite exception of measurements performed by Allard's group). Fortunately, better attention has been paid to such factors when performing measurements over the last decade. Nevertheless, gaps still exist, and for several elements few sorption data are available.

Carbol and Engkvist (1997) acknowledge that the focus of much of the experimental data has been on Swedish research institutes and the reasons presented for relying on

such data (relevant rock-water systems, ability to compare similar element behaviour) are justified.

1.2.3 Effect of Humic Substances

For SKB 91, Allard *et al.* (1991) modified the recommendations of Albinsson (1991) to take account of the possible effects of natural organic (humic and fulvic) acids. Such material was assumed to complex with the metal ion, forming low-sorbing complexes above the point of zero charge for the rock/mineral surface. Reduction by a factor of 2 was recommended for most cations (except Cs), but by a factor of 10 for trivalent elements, although no experimental data were used to support the reductions. Allard *et al.* (1991) used as an estimate for the concentration of humic substances of 10^{-4} kg/m^3 (maximum value $5 \cdot 10^{-4}$ kg/m^3), a factor of 10 less than the *total* organic concentrations adopted by Carbol and Engkvist (1997) for the deep Swedish groundwaters. Carbol and Engkvist (1997) note, however, that the concentration of humic substances is typically about 15% of the total dissolved organic carbon (DOC), so the relevant concentrations are similar in both cases.

Even with the same concentration of humic substances, there is some discrepancy between the conclusions of Allard *et al.* (1991) and Carbol and Engkvist (1997) which merits some discussion. Bruno and Duro (1997) do not address the possible effects of such organic material in solution.

Experimental data for radioelement sorption in the presence of low concentrations of humic acids do exist for actinides (Am, Pu) and trivalent elements. For example, Labonne *et al.* (1992) provided experimental evidence supported by surface complexation modeling, of a reduction in the sorption of Am on silica in the presence of humic acids in the range 1 to 10 mg/l. Reduction by a factor of at least 10 was noted. Similar results have been reported by Nedén *et al.* (1994) for the sorption of Eu on alumina at neutral pH. On the other hand, Wei *et al.* (1998) noted the formation of Eu-humate complexes (humic concentrations about 150 mg/l) but subsequent strong sorption of these complexes. Therefore, conflicting reports exist even in the recent literature!

Provided the concentration of humic substances is < 10 mg/l, the decision by Carbol and Engkvist (1997) that the effects of such low concentration of humic substances are negligible is probably a reasonable one. However, the possibility of higher organic concentrations could be accommodated with respect to trivalent and certain actinides (*e.g.* Am) by increasing the uncertainty range for such radioelements. Certainly, organic concentrations should continue to be monitored to ensure that concentrations do not exceed 10 mg/l.

1.2.4 Ionic strength

There is a slight inconsistency between the boundary between non-saline and saline of Carbol and Engkvist (1997) and Ohlsson and Neretnieks (1997). The former selected 500 mg/l of chloride as the limit for non-saline and 500 mg/l to 6500 mg/l as saline reference groundwater, based on detailed work of Laaksoharju *et al.* (1998), whereas Ohlsson and Neretnieks (1997) used a salt concentration of 1000 mg/l as the limit below which is low salinity water but 10,000 mg/l as the lower limit for high ionic strength. In effect, both sets of authors treat the same reference waters as either low ionic strength

(non-saline) or high ionic strength (saline), *i.e.* high ionic strength and saline are the same category, so no discrepancies should be generated by the above inconsistency. Much, however, depends on the salinities used as the basis for compiling/reviewing experimental data on sorption and diffusion.

The suggestion by Bruno and Duro (1997) to use one range of K_d values for saline and non-saline groundwaters may well be prompted by the experimental data, but contradicts the underlying scientific basis that for elements that sorb by ion exchange, competition for sorption sites would reduce the extent of sorption in the case of a saline groundwater. In this context, the decision by Andersson (1999) to retain the differences recommended by Carbol and Engkvist (1997) is consistent.

1.2.5 Effect of Temperature

Theoretically, sorption is expected to decrease with increasing temperature, all other variables being constant. However, few data have been collected at elevated temperature and the results from these experiments are often conflicting, primarily because the chemistry of the solid-liquid-phase system does not remain constant, but is affected by the increase in temperature.

Ames and coworkers (1983a, 1983b) carried out measurements on individual minerals at elevated temperature. Unfortunately, their results are inconclusive in demonstrating the influence of higher temperature (some K_d values higher, some lower with higher T). The authors attribute some of the variability to changes in the solid phase (minerals) brought about by higher temperature.

Baston *et al.* (1999) recently presented measurement data involving the sorption of Ac and Pa on bentonite, tuff, and granodiorite at 20 C and 60 C. These researchers noted a difference in K_d values depending on filtration technique, suggesting the presence of 'particulate' material (polymeric species). However, after ultrafiltration, the K_d values for Ac and Pa at 20 and 60 C were similar. In this case, the presence of polymeric species is an additional 'complication'.

1.2.6 Nature of Solid Phase

K_d values are very much dependent on the rock-water system being studied. In the work of Carbol and Engkvist (1997), less emphasis was placed on the nature of the solid phase (granitic rock) compared with the groundwater composition. With respect to the rock, or solid phase, Carbol and Engkvist (1997) considered that the same highly-sorbing component minerals are present in most crystalline rocks, although the individual quantities may vary.

Carbol and Engkvist (1997) choose to ignore difference in experimental data between intact and crushed rock samples. On balance, this is reasonable since expected differences are expected to be less than a factor of 3.

1.2.7 Non-linear Sorption

Non-linear sorption has been demonstrated for certain elements, though normally at concentrations above those found in deep natural waters. Nevertheless, the conclusion of Carbol and Engkvist (1997) to ignore any change in K_d for Cs with Cs concentration

is acceptable *for the Cs concentrations of relevance to the SFL repository*. Such a decision should not, of course, be made unilaterally (for the Swiss crystalline groundwaters, for example, some consideration had to be given to non-linear sorption, as discussed in Stenhouse, 1995).

1.2.8 Thermodynamic Data and Speciation

Speciation diagrams are frequently prepared to show the predominant species for a particular radioelement. While such diagrams are useful for showing the dominant species, no account is taken of the potential role of the solid phase for affecting the equilibrium position. Thus, for example, where there is a strong preference for the sorption of one particular type of species of a radioelement, some redistribution of aqueous phases is expected due to a disturbance the equilibrium.

1.2.9 Editorial Comment – Internal Consistency

The ranges quoted in Table 12-1 of Carbol and Engkvist (1997) for Cd, though expected on the basis of chemistry (saline *vs.* non-saline conditions) do not match the recommendations in Section 12.4.3, page 48 of the same report.

2.0 Sorption Data for Compacted Bentonite

The following references were reviewed in detail:

- *Section 5.3,* Andersson (1999);
- Yu and Neretnieks (1997);
- Ochs (1997);
- Olsson and Neretnieks (1997)

Extracts from other references quoted below were reviewed as discussed in the text.

2.1 General Review Comments

Radionuclide transport through the bentonite buffer is taken into account via diffusion, with sorption where merited. The input parameters required, therefore, are effective diffusion coefficient, D_e, distribution coefficient, K_d, and porosity, e. Andersson (1999) notes that the code used to model migration through the near field can use only one value of porosity, which leads to logistical problems regarding data input. In particular, K_d values must be 'manipulated' to yield a D_e value representative of the transport porosity and the true sorption capacity for that radionuclide. In this regard, comparison of K_d values with other programmes must be treated with caution.

The reference conditions for bentonite adopted by Yu and Neretnieks (1997) included a dry compaction density range of 1600-2000 kg/m^3. The starting point for their work was the previous set of recommendations for SKB 91 by Brandberg and Skagius (1991). Ochs (1997) carried out a review of the recommendations of Yu and Neretnieks (1997). Relevant sets of data are provided in *Table 2*. For the diffusion/sorption data base for bentonite, Andersson (1999) appears to have taken into account all the (conservative) recommendations proposed by Ochs (1997).

In providing recommendations of K_d values, Yu and Neretnieks (1997) did not identify a reference porewater composition for compacted bentonite, which seems a major omission. The omission may well have been influenced by the lack of a consensus in how to establish a reference porewater composition (see Section 2.2.1).

It is now well established that K_d values obtained from batch sorption experiments must be treated with caution. The comment by Ochs (1997), that K_d values cannot and should not be evaluated independently of the diffusion model used (*i.e.* with or without surface diffusion), is also valid. Thus, given that the near-field release code COMP23 applies a traditional diffusion model, the data input should be consistent with this model.

The main themes discussed at a recent Workshop on solute transport in compacted bentonite included (Huigi and Apted, 1998);

- the structural and chemical inhomogeneity of the compacted bentonite,
- the process of radionuclide sorption on bentonite, and
- the postulated process of surface diffusion.

With regard to sorption, it is now clear that batch sorption measurements used to measure sorption coefficients in disaggregated bentonite samples effectively ignore the

partially mobile fraction. Erroneously high (non-conservative) batch K_d values result in calculated values for D_e for bulk intact bentonite which are, in turn, too high.

In justifying the selection of K_d value recommendations, Andersson (1999) makes a series of assumptions and arguments which are clearly stated and sensible.

The topic of surface diffusion in compacted bentonite continues to generate heated debate, which has still not been resolved by recent experimental or theoretical methods. Two principal stumbling blocks with respect to compacted bentonite remain (Huigi and Apted, 1998):

- Measurements of apparent and intrinsic diffusion coefficients show a significant decrease with increasing compaction. However, the number of bulk diffusion pathways should decrease with compaction, whereas surface diffusion pathways, if they exist, should not change and so, if surface diffusion is large compared with bulk diffusion, there should be no decrease with increasing compaction.
- Several interpretations of surface diffusion have relied on Cs sorption data. In these case, the sorption of Cs was assumed to be linear but will be non-linear in bentonite, i.e. varying with porewater concentration.

Experimental data show that the effective diffusion coefficient is clearly related to the volumetric water content (roughly analogous to compaction density) of the bentonite sample, decreasing in a regular but highly non-linear manner with decreasing water content.

One of the main conclusions from this Workshop was that "*batch sorption experiments can no longer be assumed to yield conservative K_d values for the bentonite; they should be superseded by direct measurements of apparent and effective diffusion coefficients made on the same compacted bentonite sample*" (Huigi and Apted, 1998). In addition, the need for a database of well-documented diffusion (apparent and intrinsic) and sorption data was recognized.

2.2 Detailed Comments

The main comments concern the bentonite porewater composition and its effect on radioelement sorption.

2.2.1 Porewater Composition

For the input to the work of Yu and Neretnieks (1997), the lack of a reference porewater composition for compacted bentonite seems a major omission. Cho *et al.* (1995) emphasise that an understanding of the porewater chemistry in compacted bentonite is essential for the prediction of the release of radionuclides from a nuclear waste repository. Cho *et al.* (1995) found that the pH increased during squeezing experiments, settling close to 9 at 2.0 Mg/m^3. Concentrations in the porewater were lower than in the external water. With saline water, the steady-state pH was slightly lower, about 8.7.

On the other hand, the pH calculated by Ochs (1997) for bentonite porewaters was much lower, just below 7. The lower pH value was obtained by treating the system as closed with respect to CO_2 removal. The major conclusion from Ochs (1997) is that the bentonite components appear to determine the final porewater composition, whereas

calculations carried out by Bruno *et al.* (1997) suggest the opposite, that the porewater composition is reflected more by the composition of incoming (ground)water. The pH determined by Bruno *et al.* (1997) from model calculations was close to 9.

TABLE 2: Comparison of Da (m2/s), De (m2/s) and Kd values (m3/kg) on bentonite, dry compaction density 1600-2000 kg/m3

Radio-element	Brandberg and Skagius (1991) *			Yu and Neretnieks (1997)				Ochs (1997)		COMMENT
	De	Kd (m3/kg)		Da	De	Kd (m3/kg)		Kd (m3/kg)		
	(m2/s)	*Best estimate*	*Conservative*	(m2/s)	(m2/s)	*Realistic*	*Conservative*	*Realistic*	*Conservative*	
C (inorganic)	1.00E-10	0	0	5.00E-12	1.00E-12	0	0	0	0	Ochs (1997): need to consider methane also
Cl	2.50E-12	0	0	2.00E-11	1.00E-12	0	0	0	0	Ochs (1997): need higher D at higher T
Ni	1.00E-10	0.5	0.1	5.00E-12	1.00E-09	0.1	0.02	0.1	0.02	Lower Kd values cf. B&S (1991)
Se	1.00E-10	0.003	0	1.00E-11	7.00E-11	0.003	0	0.003	0	
Sr fresh	2.50E-08	0.5	0.1	2.00E-11	2.00E-08	0.5	0.1	not relevant		Ochs (1997): only one (saline) value of De
saline	N/A	0.01	0.001	2.00E-11	5.00E-10	0.01	0.001	0.01	0.001	should be used.
Zr	1.00E-10	2	0.2	1.00E-14	5.00E-11	2	0.2	2	0.05	Ochs (1997): large uncertainty in cons. Kd
Nb	1.00E-10	0.2	0	1.00E-12	5.00E-10	0.2	0	0.2	0	
Tc (IV)	1.00E-10	0.1	0.01	2.00E-12	5.00E-10	0.1	0.01	0.1	0.01	
Tc (VII)	2.50E-12	0	0	2.00E-12	1.00E-13	0	0	0	0	
Pd	N/A	N/A	N/A	5.00E-12	1.00E-10	0.01	0	0.01	0	
Ag	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	Andersson (1999): Kd=0
Sn	1.00E-10	3	0.01	1.00E-14	7.00E-11	3	0.01	3	0.01	
I	2.50E-12	0	0	5.00E-11	3.00E-12	0	0	0	0	
Cs fresh	2.50E-08	1	0.2	5.00E-12	6.00E-09	0.5	0.2	not relevant		Ochs (1997): only one (saline) value of De
saline	N/A	0.05	0.005	5.00E-12	6.00E-10	0.05	0.005	0.05	0.005	should be used.
Pb	1.00E-10	0.5	0	1.00E-12	1.00E-09	0.5	0	lower at pH < 7		
Ra fresh	2.50E-08	0.5	0.1	2.00E-11	2.00E-08	0.5	0.1	not relevant		
saline	N/A	0.01	0.001	2.00E-11	5.00E-10	0.01	0.001	0.01	0.001	
Ce	1.00E-10	1	0.2	1.00E-13	2.00E-10	1	0.2	1	0.2	
Sm	1.00E-10	1	0.2	1.00E-13	2.00E-10	1	0.2	1	0.2	
Ho	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	Andersson (1999): Sm=Ho
Th	1.00E-10	3	0.1	1.00E-14	7.00E-11	3	0.1	3	0.1	
Pa fresh	2.50E-08	3	0.1	1.00E-12	7.00E-09	3	0.1	not relevant		Ochs (1997): only one (saline) value of De
saline	N/A	3	0.1	1.00E-12	7.00E-10	0.3	0.01	0.3	0.001	Ochs (1997): large uncertainty in cons. Kd
U (IV)	1.00E-10	3	0.1	2.00E-13	5.00E-10	1	0.01	1	0.01	
U (VI)	N/A	0.05	0.005	1.00E-12	1.00E-10	0.05	0.005	0.05	0.005	
Np (IV)	1.00E-10	3	0.1	2.00E-13	1.00E-09	3	0.1	lower	lower	
Np (V)	N/A	0.05	0.005	1.00E-12	5.00E-11	0.02	0.005	0.02	0.005	lower realistic Kd cf. B&S (1991)
Pu red	1.00E-10	3	1	5.00E-14	3.00E-10	3	1	3	1	Ochs (1997): include oxidising conditions
ox	N/A	3	1	N/A	N/A	N/A	N/A	0.01	0.005	for consistency; Da should be higher
Am	1.00E-10	3	1	1.00E-14	7.00E-11	3	1	3	1	Ochs (1997): 3 and 1 values too close
Cm	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	Andersson (1999): Am=Cm

N/A = no entry or not applicable

Brandberg and Skagius (1991) provide only one value for De.

Muurinen and Lehikoinen (1998) carried out experiments on the equilibration of varying amounts of compacted bentonite with equilibrating solution (fresh and saline groundwaters) under anaerobic conditions, and concluded that the porewater chemistry is determined by a combination of:

- readily-dissolving components (accessory minerals calcite and gypsum) present in the bentonite,
- ions from the incoming groundwater.
- ion-exchange processes involving cations in montomorillonite and those in the equilibrating water.

Importantly, concentrations of species in porewaters and equilibrating solution depended strongly on bentonite:water (b/w) ratio, ionic strengths of both waters increasing with b/w ratio. The pH of porewaters was higher than in the incoming water, depending only slightly on bentonite:water ratio. The results of Muurinen and Lehikoinen (1998) indicate a final porewater pH of around 9 and 8.8 for interaction with fresh and saline waters, respectively.

Bruno et al. (1999) carried out modelling calculations involving the "instantaneous equilibration" of bentonite with three different groundwater typical of granitic waters in Sweden. Their results for all three groundwaters show a final pH of around 7, in agreement with the calculations of Ochs (1997).

Bruno et al. (1999) then modelled porewater *evolution* as a function of replacement of porewater by incoming groundwater. These authors identified calcite and pyrite as key accessory minerals in terms of porewater chemistry evolution and demonstrated that calcite constitutes the main alkalinity buffering component of the bentonite-groundwater system. Furthermore, Bruno et al. (1999) modelling results showed that porewater pH remained above 9 for at least a million years due to the alkalinity buffer being active for this time.

As one example of the influence of porewater composition on sorption properties, Ochs (1997) notes that the sorption behaviour of Pb is highly dependent on pH. Thus, in view of the lack of a reference porewater composition, the values selected for K_d should reflect this dependency (in fact, this uncertainty is covered by a zero value for pessimistic).

Given the absence of a reference porewater composition, Andersson (1999) takes note of the findings of Bruno et al. (1999) and adopts K_d values representative of saline waters with a pH above 8 (*i.e.* CO_2 removal, which is probable). Although a relatively high pH was predicted by Bruno et al. (1999) for one of the groundwaters (Gideå), Andersson (1999) notes that the impact of a pH outside the range of pH considered but on the high side, will be much less than that of a pH outside the range of pH considered but on the low. Side. Again, this assumption is reasonable.

Thus, the recommendations of Andersson (1999) for Kd values for sorption on compacted bentonite are considered reasonable.

2.2.2 Experimental data

In terms of experimental work on sorption of radioelements on compacted bentonite, effective (intrinsic) and apparent diffusion coefficients should ideally be carried out on the same compacted bentonite sample. Any variation of this approach should be interpreted with caution.

2.2.3 Inorganic carbon and methane

Diffusion of carbon as methane, *i.e.* via the use of a D_a value for methane as discussed by Ochs (1997), does not appear to have been taken into account in the database in Andersson (1999). If so, this issue needs to be resolved,

References

Albinsson Y. (1991): Sorption of radionuclides on granitic rock. SKB Working Report AR 91-07.

Allard B., Karlsson F. and Neretnieks I. (1991): Concentrations of particulate matter and humic substances in deep groundwaters and estimated effects on the adsorption and transport of radionuclides. SKB Technical Report TR 91-50.

Ames L.L., McGarrah J.E. and Walker B.A. (1983a): Sorption of trace constituents from aqueous solutions onto secondary minerals. II Radium. Clays and Clay Minerals **31**, 335-342.

Ames L.L., McGarrah J.E. and Walker B.A. (1983b): Sorption of uranium and radium by biotite, muscovite and phlogopihite. Clays and Clay Minerals **31**, 343-351.

Andersson J. (1999): SR 97: Data and data uncertainties. Compilation of data and data uncertainties for radionuclide transport calculations. SKB Technical Report TR-99-09.

Baston G.M.N., Berry J.A., Brownsword M., Heath T.G., Ilett D.J., McCrohon R., Tweed C.J. and Yui M. (1999): The sorption of polonium, actinium and protactinium onto geological materials. Mat. Res. Soc. Symp. Proc. **556**, 1107-1114.

Brandberg F. and Skagius K. (1991): Porosity, sorption and diffusivity data compiled for the SKB 91 study. SKB Technical Report TR 91-16.

Bruno J and Duro L (1997): Discussion of data uncertainties. Review of selected sorption data of radionuclides in granitic rock. SKB Report U-98-06.

Bruno J., Arcos D. and Duro L. (1999): Processes and features affecting the near-field hydrochemistry. Gorundwater-bentonite interaction. SKB Technical Report TR-99-29.

Carbol P and Engkvist I (1997): Compilation of radionuclide sorption coefficients for performance assessment. SKB Report R-97-13.

Cho W.J., Lee J.O., Hahn P.S. and Park H.H. (1995): Hydraulic and diffusive properties of clay-based backfill material for a low- and intermediate-level waste repository. Mat. Res. Soc. Symp. Proc. **353**, 299-306.

Heer W. and Smith P. (1998): Modelling the radionuclide migration experiments at Grimsel. What have we learned? Mat. Res. Soc. Symp. Proc. **506**, 663-670.

Huigi M. and Apted M. (1998): Report on "Workshop on Solute Transport in Compacted Bentonite". Mat. Res. Soc. Symp. Proc. **506**, 1101-1103.

Laaksoharju M., Hurban I. And Skarma C. (1998): Summary of hydrochemical conditions at Aberg, Beberg and Ceberg. SKB Technical Report TR 98-03.

Labonne N., Moulin V. and Stammose D (1992): Actinide sorption onto silica in the presence of humic substances: proposal of retention mechanisms. Mat. Res. Soc. Symp. Proc. **257**, 307-314.

Muurinen A. and Lehikoinen J. (1998): Evolution of the porewater chemistry in compacted bentonite. Mat. Res. Soc. Symp. Proc. **506**, 415-422.

Nedén M., Ephraim J.H. and Allard B. (1994): Radiochimica Acta **65**, 265-270.

Ochs M. (1997): Review of a report on diffusion and sorption properties of radionuclides in compacted bentonite. SKB Report R-97-15.

Ohlsson Y. and Neretnieks I. (1997): Diffusion data in granite. Recommended values. SKB Technical Report TR 97-20.

SKB (1991): Final disposal of spent nuclear fuel. Importance of the bedrock for safety. SKB Technical Report 92-20.

Stenhouse M.J. (1995): Sorption databases for crystalline rock, marl and bentonite for performance assessment. Nagra Technical Bulletin NTB 93-06.

Wei J., Van Iseghem P. and Wang L. (1998): The adsorption of humic acids and europium-humate colloids onto repository components: Boom clay, bentonite and Fe_2O_3. Mat. Res. Soc. Symp. Proc. **506**, 881-888.

Yu J-W and Neretnieks I. (1997): Diffusion and sorption properties of radionuclides in compacted bentonite. SKB Technical Report TR 97-12.

The author

Mike Stenhouse is a Principal Consultant with Monitor Scientific, formerly the Denver office of QuantiSci. His first degree (B.Sc. Honours) is in Chemistry and his Ph.D. in nuclear geochemistry/environmental radiochemistry, studying the fate of nuclear weapon-produced carbon-14 in the environment. Both degrees were obtained at the University of Glasgow, Scotland. During his early professional life, he established and operated a carbon-14 low-level measurements facility at the University of Glasgow for both research and commercial purposes. Since then, Dr Stenhouse has broadened his professional interests to include environmental topics in health physics and earth science. He has over twenty years' experience in evaluating the chemical behaviour (aqueous speciation, complexation) of contaminants including recommendations for the transport properties (sorption and diffusion parameter values) of a wide spectrum of elements. His experience includes analysis and interpretation of hydrochemical data (radioactive and stable isotope data) used for site characterisation purposes, as well as the application of systems analysis to waste disposal. In the last ten years, much of his professional work has focussed on technical aspects associated with the performance assessment of deep and near-surface radioactive waste disposal concepts.

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REVIEW

Deep Repository for Spent Nuclear Fuel

SR 97 – Post-closure safety

Ove Stephansson

Division of Engineering Geology
Departement of Civil and Environmental Engineering
Royal Institute of Technology
S-100 44 Stockholm, Sweden

Introduction

The Swedish Nuclear Fuel and Waste Management Co, SKB has presented the requested safety assessment – called SR 97 - to the Swedish Government and nuclear regulatory authorities SKI and SSI with the purpose to demonstrate that the so-called KBS-3 method has good prospects to meet the safety and radiation protection requirements which SKI and SSI have specified in recent years.

The purpose of the study SR 97 is to demonstrate by means of systematic studies, that the risk for harmful effects in individuals in the vicinity of a future repository complies with the criterion stated by the Swedish regulatory authorities. According to the KBS-3 concept the spent fuel is placed in isolating copper canisters with a high-strength cast iron insert. The canisters are surrounded by high-compacted bentonite and placed in vertical boreholes drilled at the floor of tunnels at the depth of about 500 m in granitic rocks. To demonstrate the applicability of the KBS-3 concept to Swedish bedrock conditions, SKB has collected and presented geological data from three different sites.

In a letter from SKI, 2000-03-07, undersigned has been asked to review SR 97 and in particular comment about issues dealing with rock mechanics and rock engineering aspects. The major review comments are summarized in the first part of the report. A detail review is presenter in Appendix 1, which follows the chapter sequence presented in the main report of SR 97 followed by comments to the reports on Waste, repository design and sites, Processes in the repository evolution and related background reports.

Major Comments

Methodology

A method to select scenarios is missing in SR 97. SKB states that the chosen scenarios provide good coverage of future evolutionary pathways for the deep repository. This is not the case. SKB has not made full use of the established interaction matrices and the new method of THMC diagrams to generate the relevant and important scenarios and to construct the important pathways of variables and processes, either in the established interaction matrices and the presented THMC diagrams. Hence, SKB is demonstrating in SR 97 that they lack a well thought through, sound and solid method to select and evaluate scenarios for the purpose of demonstrating the safety of a deep repository for spent nuclear fuel.

The evolution of the system is presented for the components of the repository system (fuel, canister, buffer/backfill, geosphere) and the effects of four different scenarios, but time only enters into the system for discrete events or processes, e.g. description of the relative radiotoxicity and heat decay of the fuel, temperature distribution, iron exchange process, pH in buffer, redox capacity and radionuclear release at the three sites. There is a lack of method and way of describing the evolution of the complete repository system, including the major scenarios, as a function of time.

It is essential that SKB is able to:

- consider the full range of potential scenarios,
- grade the scenarios according to their significance for repository design and performance & safety assessment,

- consider whether simple engineering actions could be taken to inhibit the development of adverse scenarios.

This cannot be done with the system presented in SR 97, and so SKB do not have a full predictive capability – which is required for the engineering design of such an important and costly structure as a repository. Thus, SKB must include a procedure for satisfying the three point above. The methodology of interaction matrices and fully coupled models as outlined in the work by Stephansson and Hudson demonstrates one method of approach, based on a comprehensive analysis of pathways through the interaction matrices. This methodology enables the three points listed above to be considered.

Base scenario

In SR 97, SKB presents the cause and effect of the heat pulse for the time up to 5,000 years after deposition. This is a stage when the heat load is distributed in the surrounding rock mass and causes thermal expansion and compressive stresses around the repository and tensile stresses close to the surface. So far there has been very little attention to the effect of the cooling following the peak of the temperature. The cooling will cause a de-stressing of the rock mass in the near-field, reduction of the normal stress across some of the fractures with a favourable orientation and increased fracture aperture and groundwater flow. Effects of cooling on the THM properties of fractures (including creep) and rock mass stability need further studies.

At present, there is limited information about the response of large rock masses to large scale heating as will be the case for the repository for the first about 1,000 years. The expansion of the rock mass in the vicinity of the repository and the generation of tensile stresses close to the ground surface might generate a stress state that cause large-scale displacement along pre-existing fractures and faults close to mechanical equilibrium. Minor stress re-distributions might disturb the equilibrium and cause displacements to occur. SKB has to look for information and knowledge about the effects of large-scale heating of large rock masses on the initiation of faults and large fractures and corresponding changes of the groundwater conditions.

Climate scenario

The climate scenario includes a brief description of the climate system of the Earth and a prediction of the climate changes we are likely to expect in the next hundred thousand years. The description of the future climate is based on three climate-driven process domains 1) temperate/boreal domain, 2) permafrost domain and 3) glacial domain. SKB describes the mechanical evolution for each of the domains where crustal upwarping/downwarping is the processes likely to be the processes that occurs in the temperate/boreal domain. Here the strains are likely to be small and uniform over large areas and should not cause differential movements along faults and fault zones.

The possible evolution in the near field of a repository due to stress changes during glaciation and de-glaciation is based on the work conducted by Hansson et al. (1995) for SKI and reviewed by SKB. Here the loading to the near-field rock mass from the ice was taken from global models in the scale of kilometres and the stability was studied by means of fracture

mechanics approach. The results show that for certain stress differences at the depth of a repository fracture initiations and propagations are likely to appear.

The state of stress and rock movements during a glacial/interglacial cycle has not been fully analysed by SKB. In the future, one would expect that SKB starts modelling works with a fracture mechanics approach related to fracturing due to ice loading and provides fracture mechanics parameters from potential sites for these type of numerical models.

Rock mechanics

Geoscientific investigation material for three selected sites are presented by SKB in the technical report dealing with waste, repository design and sites. Here is missing a general overview of the geological and rock mechanical development of the respective areas and their place in space and time during the geological evolution of the Baltic Shield. This makes it difficult to rank the suggested sites based on their past, present and future geological evolution.

The rock mechanical description of the sites consists primarily of results from rock stress measurements and laboratory determinations of deformation and strength properties of drill core samples. In general, there are not enough rock mechanical data to perform a statistical evaluation of the rock mechanical parameters for the individual sites and the data collected varies between the sites which prevent proper comparison.

Rock stresses have been measured at each of the three sites. Hydraulic fracturing stress measurements have been performed at all sites. In addition overcoring stress measurements have been used at the Aberg site. Recorded stresses from the two methods show severe discrepancies, more than usual for similar campaigns at one and the same site. The problem of large discrepancies in data needs to be resolved before stress measurements are performed at future sites.

For stress measurements in general and the demand of good quality data at the future sites, there is a need for integrated stress analysis where data from different stress measurements methods (overcoring, hydrofracturing, hydraulic testing of pre-existing fractures and focal mechanism studies) are combined in an integrated stress analysis. Results from orientation of horizontal components from the stress measurements at the three sites clearly demonstrate the relatively large variation in orientation both at each site and between different sites. The relationship between the state of stress and the location and orientation of the major fracture zones is of outmost importance in a future location of a final repository.

Preliminary repository layout was constructed by SKB for each selected repository site to accommodate approximately 4,000 canisters. From rock stability point of view the deposition tunnels should be oriented parallel with the orientation of the maximum horizontal principal stress. This is one of the fundamental principles in rock engineering. However, SKB prefer to orient the tunnel axes perpendicular to the maximum stress because the fracture zones and their respect distance, the orientation of water-bearing fracture zones and the area for repository location does not allow a proper tunnel orientation with respect to the orientation of the horizontal rock stresses. The orientation of the tunnels as suggested might lead to spalling or other types of failure of the tunnels and deposition hole. There has been a number of international studies about this problem and SKB has to give this problem additional studies to form a strategy for the future orientation of tunnels and deposition holes.

The geometry of the rock blocks is governed by the size and orientation of the discontinuities. SKB states that blocks that can accommodate tunnels with lengths in the span 250 to 500 m are advantageous from a construction-related point of view. For potential sites where there are a high frequency of fracture zones the available block are likely to be small. Hence, there is a need to define the lower limit of block size and tunnel length in the future planning of a repository.

Design and construction methods

In chapter 5 of the report on Waste, repository design and sites, SKB presents site-specific adaptation of the repository. In the section about repository design, there is a lack of information about the design method that will be applied for the repository. There are no references to standard literature about rock engineering design and design methods for underground constructions. There is a need for SKB to determine the design methods as this information is independent of the selection of a finale site for a repository.

SKB advocates “Design as you go” as an active approach during the process leading up to a finished repository and claims this as being important for safety. This method of constructing underground space can be applied for structures were safety demands are not particular important. However, the method is far from being applicable for construction of a final repository of radioactive waste. The public opinion will hardly accept such a strategy. This approach is also difficult to manage for the authorities as revised plans, safety documents and control systems have to be checked and revised continuously. To some extent this approach has been demonstrated during the present construction of the extension of the CLAB facilities of SKB and has not been functioning well.

The design method “design as you go” cannot be accepted for a repository for radioactive waste. The design issues need to be sorted out beforehand. Only minor variations can be allowed at the time of excavation, e.g. the precise position of the canister holes.

Main Report

1 Purpose and premises

SKB has formulated four concrete purposes for the SR 97 study. These purposes are based on statements presented by the Swedish Government, SKI and SSI in recent years. The four purpose statements presented by SKB in section 1.2 are:

1. SR 97 shall serve as a basis for demonstrating the feasibility of finding a site in Swedish bedrock where the KBS-3 method for deep disposal of spent nuclear fuel meets the requirements and long-term safety and radiation protection that are defined in SSI´s and SKI´s regulations.
2. SR 97 shall demonstrate methodology for safety assessment.
3. SR 97 shall serve as a basis for specifying the factors that serve as a basis for the selection of areas for site investigations and deriving which parameters need to be determined and which other requirements ought to be made on a site investigation.
4. SR 97 shall serve as a basis for deriving preliminary functional requirements on the canister and the other barriers.

The way SKB has succeeded in fulfilling these statements will be commented at the end of this review.

In section 1.3 about delimitations of the study, SKB states that SR 97 deals with the long-term safety of the repository after closure and that construction and operational phases are not dealt with. Nor is SR 97 concerned with safety in connection with a prolonged open period or a partially closed repository.

In paragraph 1.4 SKB outlines the report structure of SR 97. The ambition to present the main report as a stand-by-its-own document that can be read separately from the others makes it cumbersome for the reader of the complete work to be confronted with repetition of the same text over and over. Hence, information is extracted from the basic documents and inserted and developed in the Repository, Process and Data reports, respectively. From there information is summerized in the main report and finally into the summary of the main report.

2 Safety goals and acceptance criteria

This chapter in the main report is not commented.

3 The KBS-3 system

In the introduction to the chapter about the KBS-3 concept SKB states in brief the overall philosophy regarding how the radioactive waste in Sweden is to be managed, namely:

- Long-term safety shall not require future monitoring and maintenance.
- The repository shall be designed to permit possible future measures to modify the repository or retrieve the waste.
- The long-term safety of the repository shall be based on multiple engineered and natural barriers which contribute via different functions to the repository´s total safety.

In section 3.2 about isolation – the primary function of the repository and its second paragraph about the isolation of the rock, SKB inserts a statement saying “Mechanically, the Swedish crystalline bedrock offers a long-term stable environment for a deep repository.” This statement appears too early in the study. It is the purpose of SR 97 to show that this is the case. Therefore, this type of conclusive and general statements should not appear at the beginning of the report.

4 Methodology

In section 4.1 entitled “What is a safety assessment?” SKB presents a series of possible processes and events that could threaten isolation of the radioactive waste and reaches the conclusion that ...”we are faced with analyzing the evolution of a system of coupled thermal, hydraulic, mechanical and chemical processes.” Thereafter, SKB describes three major tasks for the safety assessment and claims that the approach is general in the assessment of systems that change with time. However, in the description and illustrations (Figs. 4-1 and 4-2) of the system there is no time scale presented. The evolution of the system is presented for the components of the repository system (fuel, canister, buffer/backfill, geosphere) and the effects of four different scenarios, but time only enters into the system for discrete events or processes, e.g. description of the relative radiotoxicity and heat decay of the fuel, temperature distribution, iron exchange process, pH in buffer, redox capacity and radionuclide release at the three sites. There is a lack of method and way of describing the evolution of the complete repository system including the major scenarios as a function of time.

The execution and presentation of the five steps in the safety assessment are presented in sub-section 4.1.3. The five steps are:

1. System description
2. Description of initial state
3. Choise of scenarios
4. Analysis of chosen scenarios
5. Evaluation.

SKB makes a clear distinction between the repository system and its surroundings and claims that the safety functions are associated with the repository system. Regardless of any perturbation from the surrounding (earthquakes, fault displacement, climate change etc.) the repository should retain its isolating and retarding functions. To lend a structure to the four systems contained in the overall repository system and the coupled thermal (T), hydraulic (H), mechanical (M), chemical processes (C) and radiation-related processes, SKB has used a system to illustrate the interaction between each of the sub-systems and the surrounding repository parts. The system is illustrated in Fig. 4-3 for the buffer/backfill and its surrounding repository parts, namely, copper canister/cast iron insert and the geosphere, respectively. The new system is an extension of the Rock Engineering System (RES) for scenario development presented by Eng et al. (1994).

The new THCM interaction system is in principal based on the interaction schemes developed by Stephansson and Hudson 1993-1994 and summarised in Eng et al. (1994). The leading diagonals for each of the matrixes for buffer, nearfield and farfield are transformed to variables. These are listed on top of each diagram for the fuel/cavity, copper canister/cast iron insert, buffer/backfill and geosphere in the chapter of system description, chapter 5. The processes for each of the subsystems are in principal: radiation (R), heat (T), water/gas (H),

pressure/movements (M) and solutes (C) and are listed on the left hand side of each of the diagrams. The important interactions between the processes and variables are indicated by arrows. A single arrow indicates a one-way coupling and a symbol with two arrows a two-way coupling. In the basic document to the development of the new method by Pers et al. (1999), the original RES matrices that form the basis for the new method are presented. Variables listed in the leading diagonals of the RES matrices are almost the same as the variables in the new method.

In the original interaction matrices variables and processes have been ranked on a four-degree quantitative scale. This gave an overview of the importance of the different interactions. As stated in subsection 4.2.4 of the Main Report of SR 97 "This information has not been transferred to the system description. Instead, the long-term ambition is to quantify as many of the processes as possible, or to show that a process is of negligible importance for the evaluation of the repository under all conditions." The semi-quantitative ranking of the importance of the interactions could have been imported to the new system simply by giving the individual couplings a coloured arrow instead of presenting the individual processes in colour. Hence, as an example a very important interaction or coupling could have been presented with a red arrow. Thereby, clusters of important couplings can be identified and the diagram will give a better overview of the important couplings for each of the subsystems.

The suggested THMC diagram has one major weak point in that interactions can only be identified from neighbouring processes out of the list presented on top of each THMC diagram. An interaction never exceeds one variable. This weakness can be illustrated by the following example. We know from geohydrology and rock mechanics that there is a strong coupling between rock stress and groundwater flow. If we look up the THMC diagram in Figure 4-5 groundwater flow is only coupled with heat, groundwater flow(?), gas flow, advection, colloid formation and radionuclide transport. In the diagram rock stress has a number of couplings to intact rocks and fractures but no interaction to groundwater flow. Hence, the interaction of one variable onto another variable can not be illustrated. Similarly, the cause and effect of one process onto another process can not be represented.

One of the important capacities of the RES system is the ability to follow a certain path in the interaction matrix and thereby being able to generate scenarios. Another ability of the RES system is to study the cause and effect of perturbations affecting any of the subsystems or the repository system. These capabilities of special importance for scenario developments are lost in the new system.

Stability of any engineering system, including a final repository for spent nuclear fuel, can be analysed by means of the fully coupled model of the RES methodology as described in Jiao and Hudson, 1995.

In the introduction to section 4.4 of SR 97 SKB says "With the system of processes defined in the system description, the repository´s evolutionary pathway is determined if
a) an initial state and
b) the conditions in the surroundings (ambient conditions)
can be determined". The RES methodology can generate a pathway trough an interaction matrix and thereby one can construct a scenario based upon the existing processes and parameters. SKB never illustrates how a scenario can be developed by means of the new method with THMC diagrams. Instead SKB in section 4.4 says: "A critical step in the assessment is choosing a number of scenarios which are than subjected to analysis". Later SKB says: "In SR 97, five scenarios have been chosen for detailed analysis. The selection is

based on experience from the work with interaction matrices, the FEP database and the system description." Later in the same section SKB admits that the new system with THMC diagrams has not been fully utilised for a systematic choice of scenarios. From a first sight it seems more difficult to generate pathways, perturbations and full scenarios with the new interaction method with THMC diagrams compared with RES methodology.

5 System description; processes and variables

In this chapter SKB describes the repository system in the special format of modified interaction method that is to be used in the safety assessment. The repository system is divided into the four subsystems fuel, canister, buffer/backfill and geosphere. The variables and processes are then defined for each one of the subsystems. The variables that characterise each subsystem are listed for different processes. The fact that the processes heat, water, gas pressure, solutes and radionuclides are similar for each of the subsystems, makes the new THMC diagrams attractive. The major drawbacks are listed in section 4 of this review of the Main Report.

The overview of processes listed in sub-section 5.6.3 could have been illustrated in time history diagram where the onset of the individual processes could have been presented at estimated times. This would have fulfilled the intentions by SKB to illustrate the development of the repository system over the indicated time perspective of 100,000 years.

6 Initial state of the repository

In the introduction to the chapter SKB states that SR 97 is carried out for the specific initial state described in the chapter. In the last paragraph, SKB advocates "Design as you go" as an active approach during the process leading up to a finished repository and claims this as being important for safety. This method of constructing underground space can be applied for structures were safety demands are not particular important. However, the method is far from being applicable for construction of a final repository of radioactive waste. The public opinion will hardly accept such a strategy. This approach is also difficult to manage for the authorities as revised plans, safety documents and control systems have to be checked and revised continuously.

To some extent the suggested method "Design as you go" has been applied to the excavation of the second chamber of the interim storage for spent fuel and radioactive waste, CLAB, and the outcome has not been very successful either from the regulatory or SKB sides. Instead, the application of the method to the extension of the CLAB facilities has caused delays in the construction work.

Time zero for the geosphere description in SR 97 prevails when the repository has just been built and closed. For the safety assessment, SKB has selected three hypotetical repository sites – Aberg (Äspö), Beberg (Finnsjön) and Ceberg (Gideå). The layout of rock caverns, tunnels deposition positions in the repository system is based on principles first presented in the KBS-3 study and presented in the Repository System report and Munier et al. (1997). The factors listed to be of importance for the layout of the repository are according to Munier et al. (1997), Table 5-1 are:

a) respect distance
b) local state of stress
c) water-bearing structures
d) shape of the blocks
e) hydraulic barriers
f) flow pattern of groundwater
g) distance to SFL 3-5.

Considering the listed factors, a preliminary repository layout was constructed for each repository site to accommodate approximately 4,000 canisters. From rock stability point of view the deposition tunnels should be oriented parallel with the orientation of the maximum horizontal principal stress. This condition is also mentioned in the technical report by Munier et al. (1997). Despite this fact, which is one of the fundamental principles in rock engineering, they prefer to orient the tunnel axes perpendicular to the maximum stress because the fracture zones and their respect distance, the orientation of water-bearing fracture zones and the area for repository location does not allow a proper tunnel orientation with respect to the orientation of the horizontal rock stresses. The orientation of the tunnels as suggested might lead to spalling or other types of failure of the tunnels and deposition hole.

The Finnish waste managing company POSIVA Oy has performed several, thorough 3-D rock mechanics modelling studies where the orientation of the deposition holes and tunnels have been studied as a function of rock strength and virgin rock stresses for three different sites of granitic rocks in Finland, Tolppanen et al., (1996; 1998), and most recently Johansson and Rautakorpi (2000). The results of the studies clearly demonstrate the increase of stability for the tunnels and deposition holes for the case where the tunnels are oriented parallel with orientation of the maximum horizontal stress.

The suggested orientation of the tunnels for all three suggested sites in SR 97 might cause stability problems for the given stress magnitudes and lead to large excavation-disturbed zones (EDZ) and hence, excess rock reinforcements have to be installed during the construction phase and perhaps later removed during the backfilling to avoid stray materials.

In sub-section 6.5.9 SKB mention that site-specific data from rock stress measurements and laboratory determination of strength and deformability exist for the three sites investigated. Compared with the situation for the Finnish site selection program, SKB has not performed a stability analysis for each of the sites where the existing data of strength, deformability and virgin stress state have been applied in order to select a proper depth of deposition and orientation of deposition tunnels. This is a weak section in the SR 97 report.

Rock stresses have been measured at each of the three sites. Hydraulic fracturing stress measurements have been performed at all sites. In addition overcoring stress measurements have been used at the Aberg site. Recorded stresses for the two methods show severe discrepancies, more than usual for similar campaigns at one and the same site. The problem of large discrepancies in data needs to be resolved before stress measurements are performed at future sites.

For stress measurements in general and the demand of good quality data at the future sites, there is a need for integrated stress analysis where data from different stress measurements methods (overcoring, hydrofracturing, hydraulic testing of pre-existing fractures and focal mechanism studies) are combined in an integrated stress analysis. Results from orientation of horizontal components from the stress measurements at the three sites clearly demonstrate the

relatively large variation in orientation both at each site and between different sites. The relationship between the state of stress and the location and orientation of the major fracture zones is of outmost importance in a future location of a final repository. The expressed uncertainties about rock stresses in relation to sites selection in SR 97 is sound.

7 Choice of scenarios

According to SR 97 “a scenario is defined as the sequence of events undergone by the repository system given an initial state and specified conditions in the surroundings.”
In SR 97 five scenarios are presented of which one is the so-called ‘base scenario’. One can question if the KBS-3 repository to be built according to known specifications under present-day condition is to be named a scenario. A more proper term would be ‘base case’ or ‘initial stage’.

A method to select scenarios is missing in SR 97. In sub-section 7.3 is listed a series of important measures for achiving completeness in the choice of scenarios, in sub-section 7.3.2 the new database for FEPs are presented on which scenarios should be extracted from and finally, a comparison of scenario developments with other organisations is presented in 7.3.3. In the conclusion to the chapter of scenarios, SKB states that the chosen scenarios provide good coverage of future evolutionary pathways for the deep repository. This is not the case. SKB has not made full use of the established interaction matrices and the new method of THMC diagrams to generate the relevant and important scenarios and to construct the important pathways of variables and processes in the established matrices and THMC diagrams. Hence, SKB is demonstrating in SR 97 that they lack a well thought through, sound and solid method to select and evaluate scenarios for the purpose of demonstrating the safety of a deep repository for spent nuclear fuel.

8 Base scenario

In section 8.4 “Overview of processes and dependencies” SKB presents the main features of the process system for the base scenario. In Figure 8-2 is presented the strongest and weaker couplings and the text describes in principle the two-ways couplings for the THMC processes. In the scenario developments and the descriptions of the processes in the repository evolution each single process is described and estimated individually without much attention to the couplings between the processes.

In section 8.6 about thermal evolution in the base scenario, SKB states that the temperature on the canister surface and in the buffer may not exceed 100°C and further that the aim of the temperature calculations for the three sites are to provide input to the description of the hydraulic, mechanical and chemical processes that are dependent on the temperature. In SR 97 is presented results from a number of different temperature calculations of the near-field and the far-field, both analytical and numerical. In general, the present knowledge is that heat conduction and temperature distribution in rock masses can be predicted with a high degree of certainty and the analytical method and computer codes applied in SR 97 have been validated against each other and against laboratory and field experiments. Hence, the concluded statements of SKB in subsection 8.6.4 of SR 97 that calculations of a repository´s thermal evolution can be conducted with sufficient precision are valid and can be accepted, so also the statement in subsection 8.6.3 where SKB admits that there is a lack of site-specific thermal

data of potential sites and that the heat transfer between different media are more uncertain than heat conduction data within a medium.

The mechanical evolution of the base scenario presented in section 8.8 deals with the mechanical evolution of the canister, given the processes expected in the buffer/backfill and further the effect of rock movements on the canister. On one hand, the presented cases (Figure 8-19 – 23) for mechanical evolution of the canister from uneven swelling pressure are too simplistic. On the other hand the existing finite element codes used for calculations of the buffer response to various loading are not suited for studies of large deformations in the surrounding rock mass. This is a dilemma and indicates that there is a need for code developments to handle this particular problem. The problem is complicated as it deals with three materials (rock, clay and metals) with great differences in mechanical properties. In 1992, SKB conducted a calculation of the strength and stability of a canister subjected to a postulated displacement of 0.10 m along a horizontal fracture. The calculated collapse load was in the range 45-55 MPa. The current design has a canister strength of 80-110 MPa, respectively.

Results presented by SKB about canister strength so far demonstrates the need for recalculation of the stability for the new canister design using numerical codes that are able to handle the relatively large displacements (0.10 m) subjected to the canister. Without such code the failure mode and resulting canister shape and integrity can not be estimated in case of rock shear displacements greater than 0.1 meter.

In SR 97, SKB presents the cause and effect of the heat pulse for the time up to 5,000 years after deposition. This is a stage when the heat load is distributed in the surrounding rock mass and causes thermal expansion and compressive stresses around the repository and tensile stresses close to the surface. So far there has been very little attention to the effect of the cooling following the peak of the temperature. The cooling will cause a destressing of the rock mass in the near-field, reduction of the normal stress across some of the fractures with a favourable orientation and increased fracture aperture and groundwater flow. Effects of cooling on the THM properties of fractures (including creep) and rock mass stability need further studies.

At present, there is limited information about the response of large rock masses to large scale heating as will be the case for the repository for the first about 1,000 years. The expansion of the rock mass in the vicinity of the repository and the generation of tensile stresses close to the ground surface might generate a stress state that cause large-scale displacement along pre-existing fractures and faults close to mechanical equilibrium. Minor stress re-distributions might disturb the equilibrium and cause displacements to occur. In the early 1980s the Swedish State Power Board constructed a large rock cavern in Avesta for storage of heat water. The heat water is produced from burning waste and is pumped into a heat exchanger. The outlet from the heat exchanger warms up the water in the rock chamber during the summer months where it is stored and later pumped into the central heating system of the city during winter. The vicinity of the rock chamber was instrumented with extensometers and stress meters and there might be a learning exercise to revisit the site and learn about rock mass response to large scale heating.

In a summary section, 8.10, SKB presents the evolution of the base scenario in a time perspective, the initial 100 years, 100 – 10,000 years and time after 10,000 years. Here the main results of the safety assessments are summarised. However, additional work is needed before SKB can claim that the mechanical stresses on the canister from groundwater pressure,

buffer swelling and rock movements around the deposition hole are far from what is needed to jeopardise canister integrity and isolation.

9 Canister defect scenario

This chapter in the main report is not commented.

10 Climate scenario

The climate scenario includes a brief description of the climate system of the Earth and a prediction of the climate changes we are likely to expect in the next hundred thousand years. The description of the future climate is based on three climate-driven process domains 1) temperate/boreal domain, 2) permafrost domain and 3) glacial domain.

In section 10.9, SKB describes the mechanical evolution for each of the domains where crustal upwarping/downwarping are the processes likely to be the processes that occur in the temperate/boreal domain. Here the strains are likely to be small and uniform over large areas and should not cause differential movements along faults and fault zones.

When an ice sheet moves over the repository the vertical load on the rock mass will increase and the loading will differ over time due to the effect of the thickness of the ice sheet and the formation of a forebulge in front of the advancing and retreating ice margin. The two type of loadings will be superimposed on the virgin rock stress and generate a complex stress situation. In SR 97, Fig.10-20, three instantaneous states of the rock stresses are depicted across a major fault at the level of a potential repository. The hypothetical evolution and stress state are likely to appear in the real situation. There are also indications from seismic recordings from glaciated terrains that the seismicity diminish due to the excess of overlying ice which support the assumption of higher rock strength under the ice due to excess normal stresses in the rock mass. However, the effect of excess groundwater and the risk of hydraulic fracturing in the upper parts of the crust is less certain and needs confirmation. The only way to check the risk of hydraulic fracturing and the state of stress at the base of a glacier is to perform in-situ measurements in a glaciated terrain like Greenland or northern Canada. Today we can only speculate what might happen at the late stage of de-glaciation.

The possible evolution in the near field of a repository due to stress changes during glaciation and de-glaciation is based on the work conducted by Hansson et al. (1995) for SKI. Here the loading to the near-field rock mass from the ice was taken from global models in the scale of kilometres and the stability was studied by means of fracture mechanics approach. The results show that for certain stress differences fracture initiations and propagations are likely to appear.

In the conclusion to the section on mechanical evolution of the climate scenario SKB states that the influence of the changes of the state of stress and rock movements during a glacial/interglacial cycle has not been fully analysed. In the future one would expect that SKB starts similar modelling works as presented by SKI and provides fracture mechanics parameters from relevant sites for these type of numerical models.

11 Tectonics – earthquake scenario

The earthquake scenario aims at examine how earthquakes will affect the safety of a repository. The chapter starts with a description of the present knowledge about the global tectonics and the geology and mechanical structure of the Baltic Shield, followed by a description of the seismicity of the Baltic Shield and the surrounding areas. The group of seismologists at the NORSAR research centre in Oslo have presented continuous data about the seismicity of the Baltic Shield for a long period of time. References to their work are missing in SR 97. The group at NORSAR also have conducted a large number of seismic risk analyses for most of the large platforms in the North Sea. Their expertise might be of value in analysing the future risk of seismic induced displacements at potential sites in the Fennoscandian parts of the Baltic Shield.

The appearance, magnitudes and distribution of intra-plate earthquakes are still not understood. The seismicity has certain cluster regions, the magnitudes are low and the depth is usually rather shallow (average 20 km). In the future geodetic measurements based on satellite data might improve the present knowledge of displacements in the upper crust. A stochastic approach has been adopted in SR 97 to determine the percentage of canister holes that are subjected to fracture movements greater than 0.1 metre during a hundred thousand years time period for the three selected sites. Despite the low seismicity in south-eastern Sweden the analysis show that Aberg (Äspö) has the greatest percentage of canister failures. As stated in SR 97 report one reason is that data from the Vänern region, with its relatively large seismicity and large magnitude earthquakes is included in the data for south-eastern Sweden.
It seems that the seismicity of the area east of the Protogene zone is different from that west of the zone. Therefore, the seismicity and related risk for large rock displacements for the Äspö region needs to be re-calculated.

The analysis of the seismic risk of the Äspö area has shown that damaging earthquakes usually occur within a couple of kilometres from the repository. Therefore, the probability of canister failure is very low once a repository is located so that fracture zones big enough to accommodate appreciable earthquakes are with a margin of a couple of kilometres. Hence, within the site selection program SKB has to consider this result and extend the area of investigation to make sure that large discontinuities at large distance from the potential site have been recorded and their influence on the stability considered.

12 Discussion and conclusions

In this chapter of SR 97, SKB is summarising the results of the different scenario analyses and presents the confidence that can be attached to the results. Further, SKB admits that a strictly executed risk calculation (probability of evolutionary pathway times calculated consequence) cannot be done for a complex system such as a deep repository for hundred thousands of years. At present he THMC diagrams introduced by SKB does not allow a proper analysis of the pathways for each of the components in the overall system and therefore, a strictly executed risk calculation can not be performed. Instead, SKB has to make a general assessment of the safety of the KBS-3 method and .. “believes that the repository design that is analysed in SR 97 has achieved sufficient maturity, that our general understanding of the repository´s long-term performance is sufficiently good, and that its potential for high safety has sufficient margins to constitute a satisfactory basis for carrying out site investigations”(cit. p. 445).

The choice of scenarios in SR 97 is an expert judgement and is not based on the content in the THMC diagram or interaction matrices. If SKB prefer to continue along this line of development there is a need for a technique to generate scenarios that are based on pathways within the diagrams or matrices. This might also generate a way to perform correct risk assessments to the individual paths within a given scenario. These statements are in line with the suggested methodology for safety assessment presented by SKB in sub-section 13.5 of SR 97, namely; a) a study of the possibilities of a more systematic choice of scenarios and b) an evaluation of probabilistic calculation methods.

How different conditions in Swedish bedrock affect the feasibility of building a safe repository is described in sub-section 4.1.4 of SR 97. The analysis is performed for long-term safety and isolation, long-term safety and release consequences and finally, thermal conditions. From a strict geological-rock mechanical standpoint Aberg seems to be more favourable compared with Beberg and Ceberg for the following reasons:

1) on a regional scale the state of stress is more consistent in orientation (NW-SE) in southern part of Sweden compared to the rest of the country.
2) the load of a future glacier is less for a potential repository located in southern Sweden
3) the present and future rate of uplift and future rate of subsidence due to glacial loading is less in southern Sweden
4) south-eastern Sweden has the lowest seismicity at present
5) south-eastern Sweden will be sea-covered during most of the life-time of a repository.

However, considering the result from the canister defect scenario, long-term safety margin is smallest at Aberg and greatest at Ceberg. The poorer retention capacity at Aberg is though compensated for by the more favourable biosphere evolution on the site.

SR 97 Waste, repository design and sites, Technical Report TR-99-08

The report about Waste, repository design and sites comprises one out of three main reference reports for the Main report of SR 97. The report describes the waste, the repository design with canisters and buffer/backfill material, the three sites and the site-specific adaptations that have been made for the repository layouts. In section 4 of the report, entitled Properties of the repository sites, the geological model and the underlying rock mechanical, thermal, hydrogeological, chemical, and transport models, respectively are presented (Figure 4-2). The geological model describes the evolution of the soil cover and the underlying rock mass and also provides a geometric basis for the repository design.

Geoscientific investigation material for the three selected sites are presented but there is missing a general overview of the geological development of the respective areas and their place in space and time during the evolution of the Baltic Shield. This makes it difficult to rank the suggested sites based on their past, present and future geological evolution. The rock mechanical description consists primarily of results from rock stress measurements and laboratory determinations of deformation and strength properties of drill core samples. The content in the report has been repeated in sub-section 6.5 Geosphere in the Main Report of SR 97. Therefore, the comments to the content need not be repeated.

In sub-section 4.4.4, Uncertainties in rock mechanical properties, it is stated that laboratory determinations of the mechanical properties are not marred with any major experimental uncertainties in themselves. This is true as long as one follows the instructions presented for

suggested methods of rock material testing. At this stage of the development of a deep repository for spent nuclear fuel at the three sites selected by SKB there is a need of more testing of all the important rock mechanics parameters in order to obtain the statistical significance and variance in the data. This comment is valid for all the listed important rock mechanics parameters in the technical report by Andersson et al., 1999. To overcome some of the problems related to uncertainties due to scale-dependency, SKB has to perform rock mechanics testing at different scales and as much as possible in-situ.

In section 5 of the report, SKB presents Site-specific adaptation of the repository. In the sub-section 5.1, Repository design, there is a lack of information about the design method that will be applied for the repository. There are no references to standard literatur about rock engineering design and design methods for underground constructions.

In sub-section 5.2, Factors that influence layout, SKB lists and describes the importance of the following factors:

- Functional classification of discontinuities
- Respect distance
- Geometry of rock blocks
- Rock stresses
- Temperature
- Flow pattern.

If a functional classification of rock discontinuities are to be applied in the design process of a repository the individual classes (D1 – D4) have to be given more quantitative data (length, width, type, structural characteristics, transmissivity, stiffness, filling etc.). SKB claims that "the deposition tunnels should be oriented in such a manner that their intersection area with conductive fractures is minimised, i.e. so that the fractures are intersected at as obtuse an angle as permitted by the shape of the rock blocks" (p. 76). This rule can cause a conflict with one of the basic rules in rock mechanics that says, and which is also mentioned by SKB (p. 76), that "deposition tunnels should normally be oriented parallel to the maximum horizontal stress or at as acute angle as possible to it". The conflict of rules is apparent in the orientation of the tunnels for the repository at sites Aberg, Beberg and Ceberg where the tunnels are oriented perpendicular to the orientation of the maximum horizontal stress. SKB has to make a clear statement about the principles of ranking of these parameters in their design work.

SKB has defined the respect distance "as the distance from an interpreted discontinuity that is required to ensure that requirements on long-term safety for a canister position are met". In order to fulfil this definition SKB has to define the absolute distance between a discontinuity and the tunnels/deposition holes for the different classes of discontinuities. This definition has to consider the virgin stress state at the repository site and the orientation of the discontinuities with respect to the tunnels/deposition holes.

The geometry of the rock blocks is governed by the size and orientation of the discontinuities. SKB states that blocks that can accommodate tunnels with lengths in the span 250 to 500 m are advantageous from a construction-related point of view. For potential sites where there are a high frequency of fracture zones the available block are likely to be small. Hence, there is a need to define the lower limit of block size and tunnel length in the future planning of a repository.

Prevailing rock stresses are site specific and influences the groundwater flow and the mechanical stability of the tunnels and deposition holes. SKB states correctly that from the

stability viewpoint the tunnels should normally be oriented parallel to the maximum horizontal stress or at acute an angle as possible to it. In adopting a repository and orienting the tunnels for the three selected sites at Asberg, Beberg and Ceberg SKB does not follow this rule.

SR 97 Processes in the repository evolution, Technical Report TR-99-07

This report describes all identified internal processes of importance for the post-closure evolution and safety of a KBS-3 repository for spent nuclear fuel. As stated in the foreword, the report is the first version of a report that will be revised prior to every safety report and a first revision will follow the review process of SR 97. The material will also be linked to the FEP database of SKB.

In sub-section 4.6.4 , Mechanical interaction buffer/near-field rock, SKB describes the different processes that can effect the rock stability and overall performance of the buffer. According to SKB the swelling pressure from the buffer is transferred to the rock but is not expected to lead to significant rock movements (p. 125). However, this statement has to be verified by results of calculations or numerical modelling and in particular for the section at the top of the deposition hole and close to the tunnel floor where high stresses are known to appear. It is important to determine the maximum amount of displacements and fracture shear that is anticipated in this area and what is the likely effect of the swelling pressure on the block displacements. In addition there should be a better knowledge of the amount of bentonite penetration into the existing fractures and newly formed fractures and what swelling pressure is anticipated in the fracture, from the fracture mouth and inward to the rock mass. In total, there is a general lack of understanding of the processes at the bentonite-rock interface including the shear forces generated at the interface due to swelling of the buffer against the backfill.

Convergence of the deposition hole due to rock creep is a very slow process. However, the deformation will cause a minor increase in the swelling pressure. The estimated increase in swelling pressure by an MPa or so is probably on the safe side.

The mechanical interaction backfill/near-field rock is described in sub-section 4.6.5. Following the recommendations by Rhén and Bäckblom (ed., 1997) the backfill should have a composition of 15 % bentonite and 85% crushed rock. In the report is missing a description of the grain size distribution needed for the crushed rock in order to give the wanted properties of the mixture. The salinity of the groundwater is also reported to have a strong effect on the performance of the backfill.

The swelling pressure and weight of the backfill is suppose to act as support against rock breakout. The aim is to achieve at least 100 kPa of swelling pressure against the roof to prevent block breakouts from the surrounding rocks and piping and creep movements in the backfill. The ongoing field tests of backfill performance in Äspö Hard Rock Laboratory will give further insight into the backfill performance in a repository tunnel.

Block breakout in the roof and walls of the tunnels is a time-dependent process and is controlled by the existing fracture network, state of stress and strength properties of the rock mass. In a series of reports for SKB Pusch has made several estimations of the development of a loose zone below an imaginary arched plane in the deposition tunnel and the dimensions of the loose rock masse in the roof of the tunnel. This whole problem complex needs further

analysis. To be able to handle the time dependent processes of the stability of jointed rock masses in the roof of the tunnel and the effect of rock reinforcement from the swelling backfill new computer codes have to be developed or the existing discrete element codes have to be upgraded with subroutines that can handle time-dependent stability problems.

In sub-section 4.6.6, Thermal expansion, SKB describes what happens when the temperature changes in the buffer. The pore water pressure rises when the temperature increases. Before water saturation, the volume of the water can expand and leads to a slight increase in the degree of saturation. However, if the buffer is water saturated and the temperature increases and the volume remains constant and no leakage can take place, the pressure can increase several tens of MPa. If drainage takes place as temperature increases the pore pressure will decrease. This is a complex mechanism that needs to be studied by fully coupled thermo-hydro-mechanical models. In the time perspective of the repository, the maximum temperature in the bentonite at the canister wall is reached after about 10 years. It is estimated that the water saturation in the bentonite reaches its maximum value at about the same time. If the wetting of the bentonite is faster and precede the peak in temperature the excess pressure can develop and cause excess loading on the rock mass. Hence, the time for water saturation is a critical factor for the storage concept of KBS-3 and the intricate coupled T-H-M processes foreseen in the deposition hole needs further analysis. This is also very much stated by SKB in the section dealing with the summary of uncertainties (p.130).

Chapter 5 of the background report about Processes in the repository evolution, deals with the geosphere. Section 5.4 of the report describes the thermal processes in the geosphere. The heat from the spent fuel is transported in the bedrock principally by heat conduction in the intact rock. Numerous studies have demonstrate that the discontinuities in the rock mass have minor influence on the heat conduction. Heat convection due to groundwater transport is also of minor importance for the overall heat distribution in the vicinity of a repository.

SKB has performed a regional study about the thermal properties of crystalline bedrock of Sweden and has determined the heat conductivity, heat flow measurements and temperature determinations at 500 m depth in boreholes (Sundberg, 1995). At a depth of 500 m the virgin temperature is found to vary between 7 and 20 °C in Swedish bedrock. The final temperature distribution in a repository is governed by the geometry of the repository tunnels and deposition holes and the power density of the spent fuel. SKB has performed several analytical and numerical calculations to determine the spacing of tunnels and deposition holes to meet the required temperatures in the buffer and backfill. The results are in good agreement both at the near-field and the far-field and there are no conceptual uncertainties regarding the processes. The temperature distribution in the vicinity of the many heater tests in hard rocks, including the Prototype repository test at Äspö HRL can be used for back-calculation of thermal data for large rock masses. The calculated values can give additional confidence to temperature predictions in the future.

Section 5.6 about Mechanical processes, gives a fairly long but very elementary introduction about deformation and strength properties of rock masses. The degree of detail and the length of this section is disproportional to the amount of actual test results of rock strength and deformability that SKB has performed for the different test sites in Sweden. For example, compared with the amount of rock mechanical testing conducted for the Finnish radioactive waste program, the data presented by SKB is very limited. A large portion of the section about mechanical properties deals with strength properties and stability. SKB also points out the decisive importance of fractures for the strength of the rock masses. It is not clear from the description whereas SKB intends to apply a fracture mechanics approach to the stability of the

tunnels and deposition holes and other processes in the safety assessment. Nor is it clear how SKB intends to approach and solve problems related to the fundamental and general processes about “movement in intact rock”, “reactivation”, “fracturing”, and “time-dependent deformations” in future safety analyses.

In sub-section 5.6.4 SKB describes the processes related to reactivation-movements along existing fractures. One of the weak points in the design of a repository is the lack of strength and deformability data about large fractures and fracture zones and the influence of rock stresses and groundwater pressure on these parameters. A few years ago Ekman et al. (1997) performed a series of interesting rock mechanics tests for SKB in the deep Laxemar borehole with the intention to increase the knowledge about strength and deformability of fracture zones. The methodology used and the results obtained are very promising and worth to apply in future site investigations. However, nothing is mentioned about these results in section 5.6.4 of the Process Report although SKB states on p. 208 that: “For large fracture zones, conceptual uncertainties exist above all when it comes to stress-deformation relationship in the shear direction.”

References

Andersson, J., Almén, K-E., Ericsson, L.O., Fredriksson, A., Karlsson, F., Stanfors, R., and Ström, A., Parameters of importance to determine during geoscientific site investigation, SKB TR 98-02, Swedish Nuclear Fuel and Waste Management Co., Stockholm, 1999.

Ekman, D., Rutqvist, J., and Ljunggren, C., Determination of hydromechanical parameters down to 1340 m depth in borehole KLX02 in Laxemar, Sweden, Papers presented at Rock Mechanics Meeting in Stockholm March 12, 1997 (ed. C. Bachman), SveBeFo, Stockholm, 1997.

Eng, T., Hudson, J., Stephansson, O., Skagius, K., and Wiborgh, M., Scenario development methodologies, SKB TR 94-28, Swedish Nuclear Fuel and Waste Management Co., Stockholm, 1994.

Hansson, H., Shen, B., Stephansson, O., and Jing, L., Rock mechanics modelling for the stability and safety of a nuclear waste repository, Executive summary, SKI Report 95:41, Swedish Nuclear Power Inspectorate, Stockholm, 1995.

Jiao, Y., and Hudson, J.A., The fully –coupled model for rock engineering systems, International Journal of Rock Mechanics and Mining Science, 32:5, 1995.

Johansson, E., and Rautakorpi, J., Rock mechanics stability at Olkiluoto, Hästholmen, Kivetty and Romuvaara, POSIVA Report 2000-02, POSIVA Oy, 2000.

Munier, R., Sandstedt, H., and Niland, L., Förslag till principiella utformningar av förvar enligt KBS-3 för Aberg, Beberg, och Ceberg, SKB R-97-09, Swedish Nuclear Fuel and Waste Management Co., Stockholm, 1997.

Pers, K., Skagius, K., Södergren, S., Wiborgh, M., Hedin, A., Morén, L., Sellin, P., Ström, A., Pusch, R., and Bruno, J., SR 97 – Identification and structuring of process, SKB TR-99-20, Swedish Nuclear Fuel and Waste Management Co., Stockholm, 1999.

Rhén, I. (ed.), Bäckblom, G. (ed.), Gustafsson, G., Stanfors, R., and Wikberg, P., ÄSPÖ HRL – Geoscientific evaluation 1997/2, Results from pre-investigations and detailed site characterization, Summary report, SKB TR 97-03, Swedish Nuclear Fuel and Waste Management Co., Stockholm, 1997.

Sundberg, J., Termiska egenskaper för kristallint berg i Sverige. Kartor över värmekonduktivitet, värmeflöde, och temperatur på 500 m djup, SKB Projekt Rapport D-95-018, Swedish Nuclear Fuel and Waste Management Co., Stockholm, 1995.

Tolppanen, P.J., Johansson, E.J.W., and Salo, J.P., Rock mechanical analyses of in-situ stress/strength ratio at the Posiva Oy investigation sites, Kivetty, Olkiluoto and Romuvaara in Finland, Eurock ’96 (Baria ed.), Rotterdam, 1996

Tolppanen, P.J., Johansson, E.J.W., Riekkola, R., and Salo, J-P., Comparison of vertical and horizontal deposition hole concept for disposal of radioactive waste based on rock mechanical in situ stress-strength analyses, Engineering Geology 49, 345-352, 1998.

The author

Ove Stephansson is professor in Engineering Geology at the Royal Institute of Technology in Stockholm. He has a PhD degree in structural geology and tectonics from the University of Uppsala and is Docent in mineralogy and petrology. In 1974 he was appointed professor in rock mechanics at the Technical University of Luleå. In 1975 he started working on rock mechanics and rock engineering problems related to the Swedish program for radioactive waste storage in hard rocks. He and his research group participated in the Swedish-American research co-operation in the Stripa mine, Sweden during the mid 1970s. In the 1980s he and his research group at the Rock Mechanics Division, Luleå University of Technology performed research work about rock deformation, rock stress measurements and numerical modelling of hard rocks for the Swedish Nuclear Fuel and Waste Managing Company, SKB, Sweden. In 1992 he initiated together with the Swedish Nuclear Power Inspectorate the international DECOVALEX project about numerical modelling of coupled thermo-hydro-mechanical processes for radioactive waste disposal. A third phase of the project is now in operation and Ove Stephansson is the acting head of the secretariat of the project. In 1993 - 94 he was member of the Royal Society, London review panel for the British radioactive waste program conducted by Nirex. His scientific expertise is rock engineering and rock mechanics and in particular rock stress, strength and deformability of rock masses and modelling of thermo-hydro-mechanical processes of rocks. Ove Stephansson has published about 50 scientific papers and books about radioactive waste storage in hard rocks.

Review of SKB's Reporting of SR 97

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Sven Arne Tirén

GEOSIGMA AB
Box 894
S-751 08 Uppsala, Sweden

Contents

1. Introduction

The Swedish Nuclear Power Inspectorate (SKI) is responsible for the reviewing and evaluating the safety of planned and existing facilities where radioactive waste is to be stored or is being stored.

The Swedish Nuclear Fuel and Waste Management Co (SKB) has performed a safety assessment called SR 97 to determine the requirements on the bedrock that will host a deep repository for spent nuclear fuel as well as to investigate how repository performance can change with time.

This report focuses on how geological and tectonic conditions are dealt with in SR 97:

- how they are described,
- how they are used as input data in the safety assessment

Three different sites/bedrock environments are studied in SR 97 and these are called Aberg, Beberg and Ceberg.

A short review of SR 97 is presented here. Each section starts with a presentation of the subject. This is followed by a brief discussion containing comments and issues addressed to SKB.

Detailed comments dealing with specific questions are presented in the appendix.

2. What Is Safety Assessment?

SKB's definition of the term "safety principles for a deep repository" is presented in the third chapter of the main report. Repository safety is primarily based on isolation of the waste. A secondary purpose is to retard the transport of radionuclides from the repository to the biosphere and a third safety function is dilution and dispersion. Factors affecting these functions are the conditions existing at the repository site ("when it has just been built and closed") as well as future changes. The future evolution is a complex and interrelated function of various parameters.

The purposes of SR 97 are (SKB 1999a: Section 1.2 Purposes) to:

1. "Serve as a basis for demonstrating the feasibility of finding a site in Swedish bedrock where the KBS-3 method for deep disposal of spent nuclear fuel meets the requirements on long-term safety and radiation protection that are defined in SSI's and SKI's regulations".
2. "Demonstrate methodology for safety assessment".
3. "Serve as a basis for specifying the factors that serve as a basis for the selection of areas for site investigations and deriving which parameters need to be determined and which other requirements ought to be made on a site investigation".
4. "Serve as a basis for deriving preliminary functional requirements on the canister and the other barriers".

3. Issues concerning Bedrock Geology

3.1 Selection of Sites and Use of Geological Terms

The three sites studied are referred to as Aberg, Beberg and Ceberg and correspond to following actual sites: Äspö, Finnsjön and Gideå respectively. "These have been selected as calculations examples to reflect different conditions in Swedish granitic bedrock…" (A page 18) and because "The sites represent three areas in stable geological settings" (A page 93).

The three sites have in common the fact that they are situated along the eastern coast of Sweden. The sites are at a distance of about 340-350 km from each other. Äspö, located 225 km SSW of Stockholm, is the site of SKB's Hard Rock Laboratory and detailed investigations have been in progress there since 1987. Finnsjön, located 115 km north of Stockholm, was included in the KBS study site programme (1977-83) and was subsequently the site (only the northern part) for the characterization of a horizontal fracture zone (1985-92). Gideå, 465 km north of Stockholm was a study site in the KBS-3 investigations (1981-83) and, subsequently, a few limited borehole studies were conducted at this site.

The dominant rock type of the different sites varies from foliated granodiorite at Aberg, gneissic granodiorite in Beberg to veined gneiss (sediment gneiss) at Ceberg. None of the sites are dominated by granite (in the strictly petrographical sense). All of the sites have a regional foliation, although this is either more strongly or less strongly developed, and they are located in three different geological terrains with different geological histories.

What is described as stable background is more a question of judgement than the classification of rock types. Sweden is situated within the Fennoscandian Shield (often called the Baltic Shield). A shield is an area within a craton where the crystalline basement is exposed, in other words, the bedrock is outcropping. Cratons are continental parts of the earth's crust that, over an extended geological period, have only slightly been affected by deformation, that is, they have not become fragmented. In a geological sense, such an area is stable. This does not mean that small-scale movements in the bedrock do not occur. "Small-scale" movements relieve the tectonic stresses that the shield is constantly subjected to. These movements can occur abruptly, leading to earthquakes or can occur without earthquakes by creep. Creep takes up most of the crustal deformation, even within the crystalline basement shields. Neotectonic movements are young movements of this type (younger than five million years old, although in Sweden, what is meant are movements that have occurred in connection with the last deglaciation or after). Knowledge of the magnitude and character of the deformation of shield areas will be considerably improved through ongoing precision GPS measurements and detailed seismic studies.

Instead of characterizing the bedrock in relation to dominant bedrock types as SKB has done, it should be related to the geological evolution of the site (the accumulated effect by superimposed processes have resulted in the present-day bedrock). The characteristics of an unfoliated granite are different in a rheological sense from a gneiss of similar chemical composition. Another example is that SKB uses the geological

meaning of the concept, such as stable area (taken from the geological definition of craton and crystalline basement shield, see above), without explaining the meaning of the transferred concept. This could be controversial and affect the general understanding of the bedrock characteristics. Movements in a crystalline basement shield are normal. However, their frequency is considerably lower than at plate tectonic boundaries.

3.2 Scales – Resolution - Structures

Firstly, it should be stated that there is a difference in what is meant by cartographic scales and geological scales. The map scale refers to the size of the represented area in relation to the size of the actual area (cf. model scale). The geological scale refers to the size of the studied object. In general, it could be said that structures represented on geological maps are large-scale and structures on the rock surface are small-scale. In geological descriptions of the area, analogue designations are used of the size of the area, for example, the local scale corresponds to the site investigation area while the regional scale covers the region surrounding the site investigation area.

Two geological scales are used in SR 97:

- regional scale
- local scale

One question that SR 97 does not answer is how large an area should be in order to describe the bedrock on a regional scale. How is the regional area delimited? Is the size of the regional area different for different geoscientific parameters? It should be stressed that the resolution of the data and the interpretation are important.

The two parameters, extent of study (i.e. delimitation of investigation including demarcation of study area) and resolution (including base data and study performance), supplement each other. It may be difficult to determine the general level of resolution that is necessary for regional studies. It all depends on the object that is being studied. Working on different scales makes it possible to apply the results gained during the regional studies to the local studies and to verify that the structural patterns that have been interpreted locally agree with the regional pattern. The relationship whereby ′anything that can be seen on a large scale can also be found on a small scale and vice versa′(cf. fractal theory) has long applied within structural geology. However, it is not completely clear from SR 97 how SKB uses the regional information.

The use of a semi-regional scale may be necessary in order to study the possible continuity from the local scale to the regional scale and vice versa. The occurrence of horizontal fracture zones is one example of structures that may be more easily confirmed on a regional scale. Another question is whether thin “local” structures exist that intersect larger structures at the boundaries of the local area. Furthermore, such a gradual transition from the regional scale to the local scale can explain local variations in the frequency for certain fracture orientations, for example, that a regional structure occurs as a concentration of small-scale structures on a local scale. An understanding of the occurrence and character of structures will be more obvious if the resolution of the interpretation is successively increased towards the local region.

The above reasoning leads to the question of how, for example, fracture zones can be identified and characterized on different scales. How are regional planes of weakness defined? How are they identified? Answers to these questions also provide answers to which zones are included on maps. In the case of Aberg, for example, for some of these zones, it is stated that "These fracture zones are often interpreted as having a width of hundred of metres, with a central fractured portion which can be up to ten or so metres wide". What is a fracture zone and what is wall rock that has been affected by processes other than fracturing (cf. for example, ductile shear and hydrothermal alteration of all rock)? It should be possible to present the structural data in the form of a structural map showing the traceable length of the structures and their thickness. An improved visual impression would be obtained if this pattern were presented in three dimensions. This would also have the advantage of making it easier for laymen to understand the existing conditions.

The fact that models are based on a gradual development of a basic model can lead to difficulties in tracing data. For example, what is the source of the information that certain regional zones in the sea outside Aberg are water conductive?

What is the relationship between topographical relief, soil depth, the level of the ground surface in relation to the base of erosion and the character of identified zones? One or two kilometres west of Ceberg, a significant elevation of the top constant of the area occurs (about 100 m difference in altitude). The importance of the structure/those structures along which this difference in altitude occurs is not explained.

The question is whether it is sufficient to have two levels of ranking for regional scales as SKB has done. Normally, a three-point scale (cf. ranking of processes for safety assessment in SR 97) is used or a scale system that handles "intermediate classes" is used. In order to do this, SKB should adjust the interpretation methodology. In short, this adjustment means that the result should determine the classification of structures and not that the classification should be determined before the interpretation is performed. Based on primary data (such as elevation data, aerial photographs) a high-resolution interpretation is obtained, representing a base map. Structural patterns in this interpretation are thereafter classified and described. A generalization can then be made based on what the presentation is to illustrate and the classification made. The result will be a thematic map.

3.3 Primary Data, Base Data and Interpreted Models

Primary data are recorded data, measurements and observations (cf. the concept data acquisition). Measurements are generally reproducible. Observations are, for example, visual recordings of relationships and are dependent to some extent on the experience of the person making the observation. In this case, base data represent data used as a basis, input data, when constructing different types of geological models, such as maps, profiles and three-dimensional descriptions. In turn, these models are the base data for planning the repository layout and groundwater transport, for example. Models that include repositories are used as a basis for calculating the migration of radioactive substances to the biosphere in the canister defect scenario. Primary data and models are used in various combinations as input data for the characterization of an area and in different parts of the safety assessment.

The geological and structural-geological presentation of the three sites varies considerably. This lack of structure for the data that are presented makes it difficult for the reader to understand, which data are relevant for the safety assessment. In addition, the level of detail in the investigations conducted at the different sites varies both in terms of the degree of detail and the size of the volumes investigated. The three sites have been investigated by different teams which have not co-ordinated the methodology for data collection and interpretation.

One purpose of SR 97 is to "serve as a basis for specifying the factors that serve as a basis for the selection of areas for site investigations and deriving which parameters need to be determined and which other requirements ought to be made on a site investigation". Furthermore, the concluding chapter of the Main Report "Discussion and Conclusions" states that the "site investigation programme includes more than the information sought by the safety assessment, however. The investigations are supposed to provide a basis for general geoscientific understanding, and many investigations do not in themselves furnish direct data for analyses, but are used when data are to be interpreted. These questions are also dealt with and discussed when the site investigation programme is formulated". More detailed information on this question will be presented later in 2000 when SKB presents its site investigation programme. This means that SKB has not given the reader a detailed view of what SR 97 has contributed on this issue.

In order to evaluate certainty/uncertainty, traceability and reproducibility of geological and tectonic models presented in SR 97, the background reports must be reviewed. Such an evaluation is beyond the scope of this review.

3.4 Repository Design

The following conditions and prerequisites determined by SKB apply to SR 97:

- "respect distance" – depends on the nature of the adjacent zone
- in this case, "In all analyses, the least favourable tunnel orientation was assumed, i.e. with the tunnel axis perpendicular to the largest primary principle stress" (C page 213)
- "Blocks that can accommodate tunnels with a length in the span 250 to 500 m are considered advantageous in the design process" (D page 76).

It would have been helpful if a diagram had illustrated the text concerning the impact of different types of zones on the repository layout. Furthermore, it would have been helpful if zones within the investigation sites had been classified according to function (class D1-D4: B, table 5-1; Almén et al., 1996) in the diagrams presented. One requirement is that the entire model area should be shown for all sites (in the case of Aberg, only the repository site, not the geographical location, is shown) so that the position of the repository is clear. A further condition should be made for repository siting (in addition to those specified by SKB): for a rock volume to be classified as a possible host for a repository, the rock volume must have a minimum width (in Aberg, there are repository volumes that can hardly accommodate one tunnel).

The planning of the location of a repository must be based on information concerning the quality of the rock. It is questionable whether this is so in the case of Aberg and Beberg. In both cases, few boreholes and the occurrence of gently inclined fracture

zones at the repository site, affect the possibility of evaluating the structural pattern in the rock at repository depth.

For each site some information presented by SKB in SR 97 have been compiled below.

Aberg

In the case of Aberg, the question is whether the rock in the southern part of Äspö is representative of the surroundings. The repository is spread out and located on two levels (a depth of 500 and 600 m respectively) and largely located outside the area where the detailed characterization was conducted. Two boreholes intersect the site where the repository is located in the upper repository level. At the lower repository level, two boreholes touch rock volumes where waste is stored. No boreholes intersect the repository volume at a depth of 600 m.

Beberg

In the case of Beberg, the northern part of the site, known as the northern block, comprises an upper less fractured unit resting on a lower more fractured unit. Between these units, there is an up to 100 m wide gently inclined deformation zone with a varying fracture frequency. The gently inclined zone has not been identified at the surface. The lower unit is assumed to have a certain similarity with the rock in the southern block. The greater part of the repository is located in the northern block under the less fractured unit below the gently inclined zone and in the more fractured domain. The rock at repository depth has been investigated by using two boreholes. Neither of these boreholes are located in rock volumes where waste is deposited. Two zones have been identified from the surface to repository depth.

Ceberg

In Ceberg the location of the repository at a depth of 500 m has been penetrated by five boreholes. In Ceberg, the size of the rock volumes where waste could be deposited is considerably larger than at the other two sites. The form of these rock volumes is very irregular. Does this indicate that structures intrude into the rock volumes (with dead ends in the rock volume) or are there structures missing in the model?

General Comments

The above description of knowledge of the rock in the areas where the repository is located should be included in the description of the repository (see also Appendix).
SKB should review the geometry of the rock volumes that will host deposition drifts.

3.5 Uncertainties

Firstly, the concept of uncertainty is examined in general and this is followed by a discussion of uncertainties in geological models.

3.5.1 General

Uncertainty is defined as “a lack of knowledge” (Andersson, 1999: Section 2.1 Uncertainty Concepts).

Uncertainty can be defined as a measure of a lack of knowledge, information and training within a particular area and the concept also includes deficiencies in specifying the relationship between cause and effect. The latter can also be expressed as an inability to be able to predict what will happen if a system is subjected to an external event.

The relationship between knowledge and uncertainty is complex and it is debatable whether or not the one is the opposite of the other.

3.5.2 Geoscientific Models

The uncertainty of the geological-structural model can be investigated by developing alternative, independent models. Doing this means, to a certain extent, that base data for subsequent models must be changed. Furthermore, the development of alternative models at each stage involves a whole spectrum of possible interpretations. Geological and structural-geological modelling can be considered to be interrelated functions, since the results may depend on the interpretation of the data quantities used, whether or not data are used in a certain order or whether data are simultaneously used. Furthermore, the modelling methodology should be described and systematically implemented. It is recommended that SKB should commission two separate groups to develop alternative models. This approach will enable characteristics to be identified in the model that are related to the treatment of data by the specific modelling group.

The question of what are the similarities and differences between the repository site and the surrounding region illustrates both uncertainties in the models and in the input data (especially with respect to representativity). Furthermore, studying the degree to which models explain and incorporate primary data and observations can assess the uncertainty in the models.

This type of information will provide some idea of the uncertainty in the models and calculations. SKB has not applied any of the three approaches to data uncertainty handling described above.

Since SKB can use alternative hydrogeological models to study possible spread in interpretations, SKB can also use alternative geological and structural-geological models to study the result (spread) that is dependent on the characteristics of the model used. SKB points out that the characteristics of input data have a greater impact on the spread of results than the hydrogeological model used. Input data in both deterministic

and stochastic models do not only comprise primary measurement data but also interpretations (such as structural geological models).

4. Conclusions

The task of the safety assessment is to show “that the repository has been designed with sufficient margins to be safe in spite of the incomplete knowledge available”. SKB mentions “confidence in the results” as an important aspect. For the layman, confidence in the information presented is of the greatest importance. This means that the presentation of the safety assessment should be of a high visual standard with respect to descriptions of processes and events.

SKB presented the purpose of SR 97 as four points (see Section 2 above, since the comments below are related to these four points). From a geological-structural geological viewpoint, the following can be mentioned:

1. Methodology for evaluating the geometry of the structural patterns of the bedrock at a depth of 500 m exists in general, but there are also certain deficiencies. Examples include determining the position of the individual structures and obtaining information. The importance of the bedrock is not completely clear. What is related to the rock type and what is related to the geological environment (including the geological evolution)? A clearer and more systematic compilation of data used in the safety assessment is required.
2. Work involving alternative models and evaluations of how well the models explain the collected data would be appropriate. The geological and structural models for a site are included as the base data in calculations and other modelling conducted in connection with the characterization of a site.
3. SR 97 does not provide any detailed information on site investigations.
4. The function of the bedrock as an external barrier is shown. However, to a certain extent, information on how this barrier can be affected by aseismic creep movements along fracture structures and the impact of selective erosion along such structures is lacking. Furthermore, criteria for properties of the rock volumes where deposition drifts are planned should be expanded, such as by determining a minimum width and suitable length-width relations.

References

Almén, K-E., Stanfors, R. and Svemar, C., 1996. Nomenklatur och klassificering av geologiska strukturer vid platsundersökningar för KBS:s djupförvar. SKB Projekt Rapport PR-D-06-029. (In Swedish).

Andersson[B], J., 1999. SR 97 Data and Data Uncertainties, Compilation of Data and Data Uncertainties for Radionuclide Transport Calculations. SKB Technical Report TR-99-09, Stockholm.

SKB[A], 1999a. Deep Repository for Spent Nuclear Fuel. SR 97 – Post-closure Safety. Main Report Volume I and II. SKB Technical Report TR-99-06, Stockholm.

SKB[D], 1999b. SR 97 Waste, Repository Design and Sites. SKB Technical Report TR-99-08, Stockholm.

SKB[C], 1999c. SR 97 Processes in the Repository Evolution. SKB Technical Report TR-99-07, Stockholm.

SKBF/KBS, 1983. Kärnbränslecykelns slutsteg. Använt kärnbränsle – KBS-3 Svensk Kärnbränslehantering AB/ Avdelningen för Kärnbränslets Behandling och Slutförvar (now known as SKB), Stockholm. (In Swedish).

In the text SR 97 references are given by letters A to D (cf. Appendix)

APPENDIX

Review of SKB's Reporting of SR 97

Contents

1. Focus and Structure of the Review

The review presented in this appendix is an expansion, and in certain cases, a clarification of information presented in the main text. In particular, this review examines certain topics in the bedrock geology and tectonics presentation in SKB's SR 97 safety assessment and how these topics have been presented on different scales (regional to local). The combined geoscientific knowledge of a site is the basis for the layout of a repository at the site. This topic is dealt with before repositories at the three different sites are discussed. Some of the parameters that can affect the future performance of a repository (scenarios) are discussed and this is followed by general comments on uncertainties in background data and interpretation. Uncertainties are also dealt with under a separate sub-heading in each section. Finally, a general overview of the impact of geological and structural geological interpretations on the safety assessment is presented.

The following issues are examined in this review:

- similarities and differences in data (how are the variations in the purpose of the investigations of the three sites and the variations in the level of detail taken into account?)
- the relationship of interpretations to interpreter, interpretation methodology and base data (input data)
- how the results are presented (what is presented and why, including traceability)
- consistency in the presentation of the sites.

The scales dealt with are:

- the regional scale (has the size of the regional scale been justified and what is the information provided by the regional study that has been used for the characterization of the local site?)
- semi-regional scale (size and the information that can be obtained for an assessment of the local site)
- local site (size and level of detail).

In the review of the repository layout, the following factors are taken into account:

- criteria for an assessment of the suitability of the rock
- how these criteria have been applied
- presentation.

The review presented here is based on parts of the following reports:

A. SKB, 1999. Deep Repository for Spent Nuclear Fuel, SR 97 – Post-closure Safety. Main Report, Volume I & II, SKB TR-99-06, Stockholm.
B. Andersson, J., 1999. SR 97 Data and Data Uncertainties, Compilation of Data and Data Uncertainties for Radionuclide Transport Calculations. SKB TR-99-09, Stockholm.
C. SKB, 1999. SR 97, Processes in the Repository Evolution. SKBTR-99-07, Stockholm.
D. SKB, 1999. SR 97 Waste, Repository Design and Sites, SKB TR-99-08, Stockholm.
E. Munier, R., Sandstedt, H., and Niland, L., 1997. Förslag till principiella utformningar av förvar enligt KBS-3 för Aberg, Beberg och Ceberg. SKB R-97-09 (in Swedish), Stockholm.

F. SKB, 1999. Djupförvar för lågt- och medelaktivt avfall. SKB R-99-59 (in Swedish), Stockholm.

G. Bäckblom, G., 1989. Guidlines for use of nomenclature on fractures, fracture zones and other topics. SKB Technical PM 25-89-007, Stockholm.

The above reports are referred to as (A), (B), (C), (D), (E), (F) and (G) below.

Only in exceptional cases have other reports been studied. When this has been done, the aim has been to understand modifications made in SR 97 of previously presented models and to obtain a clearer view of the underlying work (traceability).

Before the geoscientific content of SR 97 is discussed, some general comments are presented.

2. General Comments

2.1 Data Used

Existing regional and local data are listed in tables. However, it is not clear which of these data have been used in modelling Aberg, Beberg and Ceberg.

2.2 Text – Diagrams

The text is brief, as it should be, but in the bedrock geology sections, it has been found that the text and diagrams sometimes do not agree, e.g. the description of regional zones for Aberg and the information presented in the accompanying diagram (D, Figure 4-3). It is recommended that diagrams should be presented using one scale and consistent designations throughout (such as geological maps and vertical cross-sections as well as rock stress measurements).

2.3 References

The sources of background data are provided in the form of references and the text is supported by diagrams and tables. Referenced text often comprises summary reports or reports that have made an extra contribution to previous investigations. References to background reports and base data are often deficient.

To this must be added the fact that different reports can refer to different compilations, that is different parts of SR 97 may be based on non-identical background data (see for example, below in the rock stresses section).

3. Geological and Structural Geological Evaluation

3.1 Selected Sites

The three sites called Aberg, Beberg and Ceberg correspond to the following actual sites: Äspö, Finnsjön and Gideå (see tables 3.1 and 3.2). "The sites have been selected as calculation examples to reflect different conditions in Swedish granitic bedrock…" (A, p. 18) and "The sites represent three areas in stable geological settings" (A, page 92).

Table 3.1: Data concerning site location and rock types at the sites.

Site	**Actual Site**	**Distance to Stockholm**	**Investigated**	**Distance to Coast/Elevation above sea level (a.s.l)**	**Main Rock Type**
	Äspö: SKB's Hard Rock Laboratory, 450 m deep	230 km south	1986-to present (ongoing)	Island in archipelago 0-15 m a.s.l.	Weakly foliated granodiorite
Beberg	Finnsjön; KBS-1&-2 study site,	110 km north	1977-1983	15 km about 30 m a.s.l.	Foliated granodiorite
	Fracture Zone Project		1985-1992		
Ceberg	Gideå: KBS- 3 study site	460 km north	1981-1983	10 km about 110 m a.s.l.	Veined gneiss, migmatite

Table 3.2: Seismic data (seismic regions in accordance with A) and isostatic uplift at each site.

Site	Above the highest shore line since	Isostatic uplift today (rate)	Total uplift	Seismic region
Aberg	about 12 500 years	1 mm/year	about 200 m	Outside
Beberg	about 10 000 years	6 mm/year	about 500 m	the Gulf of Bothnia*
Ceberg	about 9 500 years	8 mm/year	700-800 m	the Gulf of Bothnia

* At the southen boundary of the Gulf of Bothnia

What the three sites have in common is that they are located along the eastern coast of Sweden and the sites are separated by a distance of about 340-350 km. The rock types at each site vary and none of the sites is dominated by granite (in the petrographical sense). At Aberg, there is mainly a mixture of various acidic to intermediary rock types (granite to diorite, granodiorite dominates) with varying grain size and type of preferred mineral orientation (foliation). The bedrock at Beberg is homogeneous, comprising gneissic granodorite. Ceberg comprises gneissic and partially melted sedimentary bedrock. The melted parts are locally concentrated, forming ′migmatite granite′ with a granodioritic composition. However, a veined gneiss is predominant. All three sites have a regional foliation, although the intensity varies. The three sites are all located in Precambrian crystalline bedrock. However, the geological history of the sites is not identical.

What is commonly characterized as ′stable bedrock′ is more a matter of judgement than the classification of rock types. Sweden is situated in the Fennoscandinavian Shield (often called the Baltic Shield). A shield is a large area of exposed basement rocks in a craton. Cratons are continental parts of the earth's crust that has attained stability, and has been little deformed for a prolonged period. That is, they are stable in the geological sense. This means that small-scale movements in the bedrock occur within the shield. "Small-scale" movements have constantly relieved the tectonic stresses that the shield has been subjected to. These movements may or may not result in earthquakes. Neotectonic movements are young distortions of the earth´s crust (less than five million years old, although in Sweden, this usually means movements that have occurred during or after the last continental deglaciation).

Table 3.2 shows that the sites have varying features with respect to the impact on the rock. This impact may also be reflected in the rock stress patterns of the site. Gideå, which shows the largest deformation, namely the vertical movement after deglaciation, also shows the least regular rock stress conditions (is most stress-relieved?).

The basis for the site selection is not directly justified beyond the fact that SKB wishes to show that sites that do not fulfil the repository site criteria have not been found. It should not be stated, as SKB does, that the three sites comprise the same rock type and that the stability conditions are similar. This review considers that the three sites – Aberg, Beberg and Ceberg – can be compared providing that the description of the site is adequate so that similarities and differences between them are clear. However, no comparison or ranking of the sites is included in SKB's SR 97.

The KBS-3 report discussed the difference in the characteristics of fractures formed in granitic rock types vs. fractures in gneissic rock types. Fractures in gneisses are usually shorter and have a lower hydraulic conductivity than fractures in granite.

3.2 Regional Characterizations

The purpose of describing regional characteristics is to determine, for example:

- characteristics and features that can occur within the detailed area
- groundwater transport pathways through the detailed area
- characteristics that can affect the future stability of the area.

Examples of such information include the homogeneity of the bedrock with respect to rock type distribution and planes of weakness.

3.2.1 Regional Area

A central question is what is meant by a regional area? Is the size of the regional area (see table 3.3) different for different parameters? How is the regional area delimited?

How are regional planes of weakness defined? How are they identified? Answers to these questions also provide answers to the zones that are drawn on maps (see also below). In the case of Aberg, it is stated that "These fracture zones are often interpreted as having a width of hundred of metres, with a central fracture portion which can be up to ten or so metres wide" (D page 31, cf. page 38). What is a fracture zone and what is the wall rock affected by processes other than fracturing (cf reactivation of plastic shear zones and hydrothermal conversion)? Furthermore, is it, for example, specified that certain regional zones in the sea outside Aberg are water-bearing (only an assumption?).

How is the relationship between topographic relief, level above the base of erosion and zone characteristics evaluated? Are two scales for regional structure sufficient? One or two kilometers west of Ceberg there is a significant vertical shift in the top constant of the area (about 100 m difference in altitude). The importance of the structure(s) along which this altitude difference occurs is not explained.

Table 3.3: Sizes of the specified regional areas for Aberg, Beberg and Ceberg.

Site	Scale	Dimensions	Size	Number of zones in the investigated site	Sea (%)
Aberg	about 1:104 170	12.5x12.5 km	156 km^2	1 longer than 10 km, 1 smaller than 3-5 km long	More than 30 %
Beberg	about 1:375 940	50x50 km	2 500 km^2	1 well-defined lineament, 1 poorly defined lineament	About 20 %
Ceberg	about 1:242 720	31.5x31.5 km	980 km^2	6 poorly defined lineaments	About 4 %

It can generally be assumed that the topographic relief is related to the structural pattern in the bedrock, the elevation of the base of erosion over geological time and the effect of the soft sediment cover. How are the low-lying areas with low relief evaluated? See also the treatment of erosion below.

What is the relationship of the regional structures to the investigated site? Is the identification of regional blocks no longer relevant to the position of an investigated site? Do the regional structural maps display the block pattern? It is common to apply a structural classification which, at the minimum, shows a structural ranking that is more

than relevant to the question at hand (a classification into three levels is considered a minimum. This partly provides an answer to a question posed above. We shall return to this issue below).

Related to the above-mentioned question is the issue of the resolution of the regional study. Is a semi-regional scale necessary? The question is warranted since many of the structures described in Aberg, for example, do not appear to be clearly related to the regional pattern (see below).

Related questions to SKB are:

- what is the connection between regional geology and local geology
- in what way has this connection been utilized when planning investigations and interpreting results?

3.2.2 Uncertainties

Uncertainties relating to regional structures mainly concern the following:

- which structures should be included (a matter of resolution and definition of the regional structure)
- width of the structures
- dip of the structures
- identification of horizontal structures.

In all of the regional models presented, structures have not been drawn in accordance with their width but in relation to their length (Aberg: "structures" with a length > about 10 km or about 3-5 km long, and in the case of Beberg and Ceberg: well-defined lineaments and poorly defined lineaments). It can be noted that for Beberg, there is a local map where the apparent width of the zones at the ground surface has been stated.

Only in the case of Aberg has the dip of the regional structures been stated. However, the uncertainty is on the order of 10° to 60°, in the case of structures that have not been bored. Why are the "vertical" unbored structures not described as having any dip distribution? Structures investigated with boreholes have a dip uncertainty of 0° to 45°. Uncertainties in dip of more than 10° for structures investigated by borehole appear to be too much (cf. G). What is the reason for this large uncertainty? One possible explanation is that SKB's assessment is that the dip of structure shows lateral variation along the structures. Furthermore, it must be noted that the occurrence of gently dipping zones has not been discussed in spite of the fact that zones of this type are described in the region (Aberg and Beberg). Why? It is possible that SKB has not identified gently dipping structures at the sites.

3.3 Semi-regional Scale

The need for a semi-regional scale, that is a scale that links the regional scale and the local scale should always be taken into consideration. This is really not a question of scale, but a question of the resolution of the investigations conducted (applies to the resolution of the data and the interpretation as well as the size, demarcation of the investigated area).

The resolution in a semi-regional interpretation would have to be such that the structures (individual structures or groupings of structures) have a traceable length of, for example, 250 m or more are detected (independently of the thickness of the structures). In the case of Aberg, examples of such structures include the fracture swarm oriented WNW-ESE as well as defined fractures oriented in the sector NNW-ESE across N-S to NNE-SSW. In the case of Beberg, it is a question of intersecting N-S structures and in the case of Ceberg, structures oriented WNW-ESE and ENE-WSW.

In the case of Beberg, such a semi-regional interpretation has been conducted. In spite of this, certain regional structures that intrude into the local area and that are included in the semi-regional interpretation have not been included in the final local model. This was commented upon in connection with SKB's treatment of uncertainties in the underlying data (B). However, the reason for this is not given.

Some probable reasons why structures identified on the regional scale are not included in the local models are proposed below. These are:

- the size and location of the local site in relation to the regional structure
- unavailability of field data (including borehole data)
- the fact that structures do not have the expected appearance and are thereby not identified
- the fact that the regional information was not fully used.

3.4 Local Scale

The local scale should have boundaries that are oriented N-S and E-W. This reduces unnecessary errors with respect to reference to the geographical north (such errors occur in the description of Aberg in SR 97, A, Figure 9-16).

The following is shown on the local scale:

- rock type distribution
- planes of weakness patterns in the bedrock.

The resolution of the work conducted varies from site to site as well as within the different sites. SKB should improve the consistency of its presentation of the sites. This is particularly the case with respect to bedrock maps displaying structures and in vertical cross-sections.

3.4.1 Size of the Investigated Site

The actual size of the investigated site (see Table 3.4), that is, the part of the site covered by surface data (mapping, ground geophysics etc.) and depth data (boreholes, core mapping, seismic measurements, radar measurements etc.) is smaller than the geographical boundaries of the site (the surface area of the site on the map). Another way of looking at this is to consider it as a form of inhomogeneous sampling. In the case of Beberg, the sampling is also inhomogeneous with respect to investigation methods (the southern block has not been included in recent investigations – borehole radar, reflexion seismics, large-scale tracer tests etc.).

3.4.2 Rock Type Distribution

In maps and vertical cross-sections describing the rock distribution within the three sites, SKB's interpretation is that tectonic structures do not have any significant impact on the rock type distribution.

The central parts of Aberg are intersected by a marked structure oriented NE-SW. Along this structure, large parts of the rock are oxidized (lost its magnetic signature). The NE-SW structure is a mylonite zone that is traceable for more than 10 km. In spite of this, the mylonite, a shear structure, does not appear to displace any lithological contacts. The question is why?

Table 3.4: Location, shape, size and number of boreholes at the investigated sites.

Investigated site	**Location**	**Shape/ Size**	**Number of boreholes (bh)**	**Concentration of bh**	**Number of bh to repository depth 500m/600m**
Aberg	Island within an archipelago	Triangle about 1 km^2	From surface: 12 From tunnel: 12 (or more?)	Central and southern Äspö	From surface: 5/2 From tunnel: 4/0
Beberg	Crystalline basement plain	Rectangle 5 km^2	From surface: 11	Central and southeastern part	From surface: 7/2
Ceberg	At the boundary of regional elevated area	Rectangle 6 km^2	From surface: 13	Central parts	From surface: 11/11

The geological map shows that the rock boundaries have a strike that conforms to foliation while in the profile, the rock bondaries are more or less horizontal and are thereby intersected by the vertical foliation. Why is this so? Is there large-scale lineation?

On the regional map of the area surrounding Aberg, the "granitic bedrock" is referred to as Småland granite while on the local map and in the local profile, it is only "Ävrö granite" that is referred to as Småland granite. Why? Is the "Äspö diorite" an exotic rock type in the region?

3.4.3 Zone Designations

The designation of structures should be simple and adequate. Some examples of inconsistent and unclear designations used in SR 97 are presented below:

- the EW-1N and EW-1S zones in Aberg comprise a zone that, according to the text and diagrams, is oriented NE-SW (A Table 6-4; according to the table, oriented in W-E to ENE-WSW; different names and different shapes are used for this zone in different background reports, although the latter is more understandable)

- zones 2A, 2B, 3A, 3B and 11A, 11B in Ceberg (A Table 6-8; alternative interpretations or real zones?; the designations of zones are not used on maps or in profiles).

It should be easy to compare zones specified in text, diagrams and tables.

3.4.4 Data for Evaluation of Uncertainty of Interpretation

To assess the uncertainty of interpretations, the location of boreholes should be included. Boreholes are indicated in vertical profiles for Aberg and Ceberg, although without specifying in any diagram the locations of these boreholes on the surface. The location of boreholes at repository depth is also essential to an evaluation of repository layout (see below).

In order to check the certainty/uncertainty, traceability and reproducibility of the models presented, background reports must be reviewed. Such work is beyond the scope of this review.

3.4.5 Presentation of Zones

The traceability of presented structures differs from site to site.

- Aberg. No maps of zones are presented. All of the zones listed in the table are not included in diagrams and there is no vertical cross-section displaying the zones The model shows the strike of structures where they intersect the main tunnel of the Äspö Hard Rock Laboratory. This type of model is mainly useful for vertical structures. Three-dimensional models are available but are not presented.
- Beberg. Mainly as a result of few boreholes and inhomogeneous rock, no check is available of the location of structures below Zone 2 in the northern block, that is, at repository depth. The check of the location of structures in the southern block is deficient. Profiles contain more structures than the structural map.
- Ceberg. This site has several structures that appear irregularly (poorly defined extensions?) and the relationship between these and other structures is unclear. Zone dip information is not specified on maps. Tabulated structures cannot be easily correlated with structures on maps and in profiles.

A consistent description of the three sites in text, diagrams and tables would make it easier for the reader to see similarities and differences between the sites.

3.4.6 Uncertainty of Interpretation

The relationship between information density and the number of identified zones is important. In the KBS study site project (six sites, including Beberg and Ceberg) systematic boring campaigns were carried out to identify and characterize target structures. About 75% of the boreholes hit the target. The relationship between the number of expected zones (targets) and structures that were shown and additional structures that were included in the models was about 1:1, that is, besides the structure to be investigated by the borehole, an additional zone occurred. In addition, somewhat less than 50% of all of the zones were bored at a depth of between 50 to 300 m, and usually at a depth of 100 to 200

m. About 35% of all of the modelled zones in these areas were investigated by a single borehole. Somewhat less than 30% of all of the zones that are included in the models were not investigated by a borehole. In the case of Aberg, the figures are different.

The above emphasizes the fact that the sampling procedure is vital in obtaining representative and homogeneous sampling. No evaluations indicating the uncertainties related to the representativity of the borehole investigations conducted within the three sites have been found in SR 97. This probably indicates that SKB has not conducted any such investigations. If this is not taken into account, the sampling of structures of specific orientations could be more comprehensive than others, in other words, this will result in an incorrect relative distribution of structures within the presented model.

Uncertainty in interpretation models can also be expressed in the share of recorded indications of planes of weakness and groundwater transport pathways that are explained by models. How much has it been possible to explain? SR 97 does not provide this type of information.

The development of alternative (independent) models could show where the uncertainties (weaknesses) in and certainties (strengths) are in the models. This would also test different approaches to modelling. In general, SKB only works with one set of geological and tectonic models and these models are adjusted as new information emerges.

Another measure of uncertainty is to study how many boreholes at repository depth pass through the rock volume containing deposition drifts. This is discussed in Section 5 “Repository”, see below. SR 97 does not provide this type of information.

SKB states for Aberg “the carefully investigated area is quite small and the question could be asked whether this volume is representative of the site condition in general. It has been suggested that the actually investigated volume is anomaly fractured, tectonised unit if its own”. “Still no new or altered structures in the Aberg structural model are suggested” (B page 54, cf. D page 45). No alternative interpretation is proposed for Äspö since the area chosen for the modelling is naturally delimited and well researched” (D page 47). Does this also apply to the immediate area where the repository is located? Note that the location of most of Aberg’s boreholes and the location of Äspö Hard Rock Laboratory’s tunnels are located has largely been classified as unsuitable for the location of deposition drifts.

It is normal for the variation/change in orientation of regionally defined structures to be relatively moderate. How well has SKB established the orientation of the “major highly conductive zones” (D Table 4-11) that intersect the southeastern part of Ceberg? The model (the vertical cross-section) states that they are perpendicular. This would appear to be unlikely since they are part of a structure that can be followed for more than 25 km (see Askling, 1997). This is a vital question since it is of fundamental importance for the interpretation of variations in the orientation of regional structures.

4. Rock Mechanics

Without being an expert in the area, I would like to raise a number of questions regarding this section. Each of the sites is then discussed.

What is the meaning of the values that are obtained from rock stress measurements? To what extent is the measured rock stress related to structural inhomogenities in the rock? What role does regional studies of rock stresses play? What type of data (rock stress measurements, interpretation of seismic data/interpreted fault plane, geodesic data) are used to assess regional stresses?

The measurements at Aberg have a distribution in direction of about 90°. How is the mean direction of the horizontal principal stress calculated when the distribution of the measurement points is inhomogeneous and the distance to the structures varies (the types of structures also vary). Are the principal stress directions expressed by some sort of "simplified" mean value?

4.1 Aberg

Since "the vertical stress is much lower than the maximum horizontal stress and agrees, at least on average, fairly well with the lithostatic load",(A) horizontal structures should have a propensity for water conductivity. However, SKB does not consider that it has observed this in Aberg. How can this be explained?

In the case of Aberg, it is stated that the most frequent orientation of water-bearing fractures is sub-parallel to the maximum horizontal principal stress and that they are vertical. This has affected the selection of the direction of deposition drifts in SR 97. However, structures that are perpendicular to the maximum horizontal principal stress have determined the boundaries in the model for rock volumes hosting the repository. Why has more attention been paid to the quantity of water-conductive fractures of a certain orientation (WNW-ESE to NW-SE) than to the more water conductive fractures but not so frequent fractures of another orientation (NNW-SSE), with respect to the choosen orientaion of deposition drifts? What is SKB's view of the interaction between these fracture sets? Do fractures of the two sets of fractures transect rock volumes hosting deposition drifts?

The references to rock stress measurements in Aberg vary in the different parts of the SR 97 reports.

4.2 Beberg

At Beberg, the measurements of the maximum and minimum rock stresses follow each other above Zone 2 while there appears to be a more irregular pattern below Zone 2. The rock stresses below Zone 2 can be divided into two groups: one with higher stresses and another with lower stresses. "Stress pairs" are thereby obtained (two pairs) that follows each other in the same way above Zone 2. The rock below Zone 2 is more fractured than above Zone 2 and is similar to the rock south of Zone 1 (that is in the southern block). Could it be so that certain parts of the rock are more stress relieved than others and that this is a function of the structural pattern of the rock? Can the spatial variation in the rock stress amplitudes indicate that the higher stresses are residual stresses? SR 97 has not dealt with these issues and neither has it taken into account the classification of rock stress.

4.3 Ceberg

Is the almost 90° rotation in the mean value for the maximum horizontal stress in relation to Aberg and Beberg caused by the relationship to the foliation in Ceberg? Does the foliation also affect the order of magnitude of the horizontal stresses? Has the considerable vertical uplift (about 800 m) at the site also affected the rock stresses?

4.4 General

A scale problem for rock stress measurements is acknowledged by SKB, although SKB does not state how this is resolved.

By using consistent diagrams (with respect to symbols, colours and scales) when presenting the same type of data from the different sites, SKB makes the text easier for the reader to understand. Deviations from this recommendation also occur in diagrams other than those dealing with rock stresses, such as diagrams describing geothermal gradients and geological maps.

5. Repository

The following terms and conditions apply (D and E) to the repository:

- "respect distance" – depends on the nature of the adjacent zone
- in this case, the deposition drift must be in the most unfavourable direction in relation to the maximum horizontal stress, that is, perpendicular to the stress
- blocks must be able to accommodate long deposition tunnels, 250 to 500 m long.

It would have been useful if the text on discontinuities had been illustrated with a diagram. In geological terminology, the term "discontinuity" is usually preceded by a qualifier (such as sedimentary, tectonic, geophysical etc.). Why has SKB introduced the term "discontinuity"?

It would have been useful if SKB had classified the zones into "functional classes" (D1-D4) in the diagrams describing the structures of the investigated sites. It would also have been useful if the entire model site had been shown for all sites (in the case of Aberg, only the repository site is shown) so that the repository location is clear.

Does SKB plan to perform pilot hole boring and to test them before boring full-scale deposition holes?

5.1 The Basis for Repository Design

In order to design a repository, adequate knowledge of the fracture pattern in the bedrock is necessary.

In SR 97, the selection of the most unfavourable direction of the deposition tunnels means that the "deposition tunnels are oriented perpendicular to the maximum horizontal stress. This direction has been chosen to avoid long intersections with water-conducting fractures that have the same orientation as the horizontal stress". (B, p. 78).

5.1.1 Aberg

The presentation of the fracture zone pattern and position of the repository in the case of Aberg is deficient. Some remarks:

- the geographical position of the repository is not specified (this also applies to the background reports – however, there is a diagram in the canister defect scenario, Figure 9-16 (A) where the arrow pointing north is incorrect). It is not clear what is considered to be the investigated site in this case
- a structural map and profiles showing the position of structures are not provided
- the repository layout is not always identical in different parts of the reports (cf. A and F)
- the entire repository layout is only provided in the F report, which is not the case in the SR 97 report.

5.1.2 Beberg and Ceberg

In the case of Beberg and Ceberg, the sites have well defined boundaries and, thereby, the geographical position of the repository is provided. However, in the case of Ceberg, the presented rock stress directions are incorrect (cf Figure 4-15 in D and Figure 6-5 in A).

5.1.3 General

Which rock stress directions have been used? They are all different from those described in "Rock-mechanical Description" (Reference D). In the case of Ceberg, the error is obvious (all sites in the diagram have the same direction of stress axes).

If the fracture orientation determines the direction of the deposition drifts why are fracture diagrams not used (stereograms, rosette diagrams or another type of diagram as well as fracture statistics) in the presentation of the investigated sites?

How and when is the methodology available for identifying suitable deposition holes?

5.2 Evaluation of the Location of Deposition Drifts

The following text on location of repositories in relation to the investigations performed has been compiled in connection with this review. The base data for this part of the present review is not included in SR 97.

5.2.1 Aberg

In connection with investigations carried out on the Äspö bedrock, different sets of structures were investigated at different times. The initial investigations focused on structures oriented in NE-SE, such as the NE-1 zone. NNW-SSE structures were then examined and these were found to have a high hydraulic conductivity in spite of the fact that the zones are very narrow and often comprised only a few discrete fractures. The fracture maps of the Äspö Hard Rock Laboratory tunnels show that the dominant fracture orientation for water-bearing (wet) fractures is WNW-ESE to NW-SE. Is there any discussion that clearly states that the latter orientation is more significant than other fracture orientations with respect to rock stability and hydraulic conductivity? In other words, why has this fracture orientation been allowed to determine the layout of the repositiory?

No map showing the location of the repository is provided in the part of SR 97 that describes the repository position (A and D: except for D Figure 9-16).

At Aberg, two of the nine boreholes that extend as far as repository depth penetrate rock volumes in the upper repository level where deposition drifts have been located. The other seven boreholes are located in rock which has been exempted due to the existence of structures and areas related to the “respect distance”. Two boreholes penetrate to the lower repository level and both are located just outside the area with the deposition hole. In brief, this means that the deposition drifts are located in areas where knowledge is deficient.

Aberg is a small island in an minor achipelago. Such islands often represent areas with a higher resistance to erosion than the surrounding water-covered areas. The narrower the channel between islands, the greater the risk that the channel will correspond to structures with low porosity, such as fracture zones. SKB writes that “the thoroughly investigated rock mass in Äspö is relatively small and may comprise an unusually heavily tectonized portion of the rock that is not representative of the entire area” (p. 47 in B). Could it be worse in parts of Äspö that are not as well investigated? Can the structures at the boundaries of Äspö island (if they exist) have an impact on the repository layout that is proposed? This can be investigated using boreholes from the lower regions of the Äspö Hard Rock Laboratory or through a three-dimensional seismic investigation (geophones placed in the TBM tunnel, at the ground surface and possibly in the lift shaft).

The occurrence of horizontal fracture zones has been discussed. During the pre-investigations, indications were found of the occurrence of a horizontal, several hundred meter wide fracture zone in the northern part of Äspö. The base of the zone is estimated to be just below a depth of 400 m and its water chemistry is different from other parts of Äspö. In the base of the KAS02 borehole (below 900 m), there is a 100 m wide section with a highly fractured rock (not included in the models?). Could this be a horizontal fracture zone?

Rock volumes where the deposition drifts are to be located should be able to accommodate drifts with a length greater than 250 m. This is rational. However, one question that should be raised is the relationship between the length of the rock volume and its width. Are the following proportions – 1:400 (width: length) or 1:10 as shown in diagrams in SR 97 – acceptable (A, see also F)? The deposition drift undermines the rock and can result in a fracture nucleus. Heat from the waste induces additional stresses. The horizontal maximum stress is dominant and is perpendicular to the thin strip of rock that contains the deposition drifts (tunnels).

Eight rock blocks used to host the repository (seven positions in the upper repository level and eight positions in the lower level. The same rock block is used for the upper and lower positions, apart from an additional block in the lower repository level). The Aberg site has four zones that are functionally classified as D1 and nine zones classified as D2. Within the area with deposition drifts, two zones are classified as D1 and six as D2. The surface of the repository is almost 1.3 km^2 on each level, in other words a total of 2.6 km^2.

5.2.2 Beberg

There is a concentration of boreholes in the eastern part of the northern block, just north of Zone 1, which separates Beberg into two parts. The boreholes are more dispersed in the southern block. At Beberg, two drill core boreholes penetrate to a depth of 600 m. Neither of these holes penetrate rock volumes where deposition drifts are located.

The greater part of the repository is located in the northern block below the horizontal zone (Zone 2). Boreholes that penetrate into this part of the rock indicate a similarity with the structural pattern in the southern block, that is a higher frequency of structures and a more complex pattern than in the rock above Zone 2.

Reflexion seismic investigations have been carried out through the northern block. What are the findings?

The repository is located in four rock blocks. Beberg has three zones which are functionally classified as D1 and eleven zones classified as D2. Within the area with deposition drifts, there is one zone classified as D1 and three classified as D2. The repository surface is about 1.8 km^2.

5.2.3 Ceberg

Ceberg has eleven boreholes that descend to a repository depth of 500 m. Five of these penetrate into rock volumes with deposition holes and six penetrate into zones at this depth.

In the version of the repository presented in the KBS-3 report, the repository is located at 600 m. Why has the repository level now been raised to 500?

Deposition drifts are perpendicular to the principal stress. However, the basis for determining this direction was uncertain as well as incorrectly positioned in the diagram (Figure 5-4 in D) and the difference between the maximum and minimum principal stress is relatively small.

The repository is located in four blocks. Ceberg has four zones which have been functionally classified as D1 and eleven zones classified as D2. In the area with deposition drifts, there are two D2 classified zones. The surface area of the repository is about 1.8 km^2.

5.2.4 Uncertainty

The reason for the performance of site investigations was different in the case of Aberg on the one hand and for Beberg and Ceberg on the other hand. The investigation of Aberg was related to the construction of the SKB Hard Rock Laboratory (Äspölaboratoriet) while Beberg and Ceberg were KBS study sites. This is reflected in the fact that the Aberg repository is split (several rock blocks and two levels) and contains most D1 and D2 classified zones. It should be noted that in the case of Aberg the model area for the repository layout is larger than Äspö itself and covers parts of the mainland (at Laxemar) as well as the adjacent peninsula (Bockholmen, northern part) and islands (Ävrö, northwestern corner and Mjälen, western part) as well as the water in between. Only a small part of the respository is located within the well investigated areas. In the case of Aberg, the repository layout must be considered to be uncertain and the value of the transport modelling must be considered in this light.

The repository layout at Beberg is uncertain since the structural pattern below Zone 2 has not been determined in detail. Beberg results in two transport models: one for the southern block with similar (homogeneous?) structural conditions and one for the northern block with a vertical contrast in the structural pattern.

The repository layout at Ceberg is the most coherent. The uncertainty in Ceberg partly stems from the irregularity of the rock block geometry and the orientation of the structures. Are there any structures that have not been identified? What is the orientation of the marked zones intersecting the eastern part of the site?

When the ability of a site to accommodate a repository is evaluated, this evaluation is based on models. One complementary alternative is to just consider primary data. The question is then whether the sampling points at the repository level indicate that a repository is feasible. However, in order to conduct such an analysis, a number of boreholes penetrating to the specific depths must exist. In the case of Aberg, Beberg and Ceberg, the share of holes through the repository site in relation to holes outside the site is as follows: 2/9, 0/2 and 5/11. Neither of these sites has a repository without intersecting zones. In the case of Aberg, individual repository areas (defined by the zone geometry and respect distance) vary from about 6,000 m^2 to just less than 200,000 m^2. In the case of Beberg, the corresponding figures are about 75,000 m^2 to just over 750,000 m^2 and in the case of Ceberg just over 60,000 m^2 to somewhat more than 1,00,000 m^2.

Should future planning of a repository be based on a degree of openness, that is that there is a possibility of adapting the repository layout to the existing conditions on a very local scale (for example, the position of the deposition drift)? In SR 97, SKB emphases that the "The KBS-3 system has a flexibility as regards repository depth and layout which allows adaption to site-specific conditions and to the information on the rock conditions which is continuously collected during site investigations and repository *excavation* (italics added by author)" (A page 445). SKB should explain the meaning of this statement.

6. Large-scale Groundwater Flow

Reference A (page 442) states that “There are several different concepts for underground water flow, and three different concepts are compared in SR 97. The conclusion of the comparison is that the natural variability of input data to the models influences the result more than the choice of model”. The questions below related to hydrogeology are outside the author’s area of competence.

Three diagrams in reference A (Figure 8-11, 8-12, 18-13) show the groundwater modelling of Aberg, Beberg and Ceberg. In relation to topographic gradients and the site size, these models are relatively deep. To show “the total flow per side” in such a model would appear to be slightly misleading since the flow can vary with depth. It is also possible that in the near-surface layer, the flow is considerably larger and in certain cases also moving in the opposite direction at a depth. In these models, shouldn’t the total flow in and out of the model volume be equal to zero? If this is not so, the changes in the groundwater level should be described as a function of time.

How is it that several different types of alternative hydrogeological modelling are performed on a single geological description of a site? Without being a specialist on hydrogeological modelling, the question can be asked whether or not there is a coupling between the different model concepts. Is there some form of calibration or basic assumption that directs the results to a specific solution? What are considered to be input data in the hydrogeological models (other models and/or registered primary data)?

If the results of the different hydrogeological models are the same for the geological-structural geological site description, why not also perform alternative structural geological site descriptions and use them as input data?

7. Scenarios

In this case, scenarios are possible processes or phenomena that can affect radionuclide migration from the repository to the human environment.

7.1 Earthquakes

An earthquake is the more or less perceptible expression of the deformation of the earth’s crust. However, only a small part of the deformation of the earth’s crust takes the form of an earthquake (more than 90% of all movements in the bedrock occur without an earthquake). This also applies in areas with ongoing mountain chain formation and along plate boundaries. To focus on where earthquakes occur at present might be incorrect. It has been found that the epicenter can move over historical time (for example, as within the Persian empire, currently Iran-Irak-Syria-Turkey). Earthquakes are only one sign that movements are occurring. Areas “without” earthquakes, such as the southeastern parts of Sweden could have the same order of magnitude with respect to deformation (both in a vertical and horizontal direction) as within areas of greater seismic density, such as

southwestern Sweden. The question is why earthquakes are more frequent in the west. The relative movement in the N-S direction is 1 mm/100 km and year (Slunga et al, 1984).

Non-earthquake related deformation, namely aseismic deformation, occurs through creep. Is this creep distributed over a large number of fracture planes or is it concentrated along a few regional planar structures? Can this deformation affect a repository? Is there any information on how creep occurs in Swedish bedrock? Is it a relative movement with alternating directions, cf indications of block movements in Finland? Is it an absolute movement for one region in relation to another, see results from the regional GPS network? The need to study aseismic movements along deformation zones has been presented in SR 97 as a future area of research. This will be an important area for future SKB research.

7.2 Erosion

The Fennoscandinavian Shield is special. The region comprising Norway-Sweden-Finland is one of the few areas where the dominant rock type at the ground surface comprises “granite and gneissic rock types”. Perhaps not much thought has been given to the reason why this is so, since it is self-evident for us living in the region. To what degree is this outcropping due to active (in a geological time frame) erosion? How much erosion can be expected over the next million years? What is the extent of the average erosion during a glaciation? The latter question can be answered by stating that it depends on the location.A study by Lidmar-Bergström (1999) indicates that the glacial erosion during the last glaciation did not have any significant influence on the landforms.

However, during a glaciation, significant, selective erosion can occur along subglacial streams and where glacier outburst floods pass. The question is, how stable the subglacial water transport pathways (channels) are with respect to their location? In areas dominated by sedimentary rock, such as in the north of Germany (extremely flat area), the North Sea and Baltic Sea, such erosion channels (incisions) are found (filled with soft sediment). The dimensions of these channels can be 300-400 m in depth, one kilometer in width and up to several tens of kilometers in length. We do not know of any such channel formations in the bedrock of the Swedish mainland. However, the possibility that they exist cannot be excluded as they can be filled with Quaternary or older sediments. In order to find out more, data from the Swedish Geological Survey’s archive on wells can be used to establish the depth to the rock surface in a valley train. Erosion of intact, sound rock by more than one or a couple of meters cannot be expected if the area has a low relief and low elevation above sea level.

8. Uncertainties

The compilation of data and data uncertainties in connection with modelling of radionuclide transport are treated in B. Uncertainty is defined as “a lack of knowledge” in B.

Uncertainty can be described as a measure of the lack of general knowledge, information and training about a particular topic, and also covers deficiencies in being able to describe

the relationship between cause and effect. The latter can also be expressed as the inability to be able to predict what will happen if a system is subjected to a particular influence.

The relationship between knowledge and uncertainty is complex and it is debatable whether they are in fact the opposite of each other.

Uncertainty relating to certain types of data has been previously dealt with in the sections where these data have been reviewed in general. A review of uncertainties relating to modelling is provided below – from uncertainties in base data (input data) to uncertainties in the model that has been developed.

8.1 Uncertainties Relating to Geological Primary Data

Uncertainty regarding the recording of geological data (primary data) may for instance depend on the following:

- What are the adequate parameters that describe the structure or what is the property of the structure that is to be investigated?
- What is the accuracy and precision with which the parameters can be described?
- What is the accuracy and precision of the location of the sample (especially in the case of three-dimensional structures - is the position of particular importance)?
- What is the spatial distribution of the sampling points (is the sampling representative)?
- What is the importance of the time sequence when sampling?

8.2 Uncertainties Relating to Geological Modelling

The evaluation of base data (parameter values obtained through sampling), namely modelling, and the presentation of results can be affected by factors such as:

- handling of data (classification/grouping of data in relation to the resolution of the base data)
- weighting of the importance of parameters
- sequence of data interpretation (how are parameters treated: separately, in a certain order, simultaneously or interactively)
- limitations of the method/methods used to interpret data (including the scale independence of structures)
- the interpretation work/modelling approach (such as interpretation procedures, consequence in implementation, boundaries/limitations)
- reproducibility
- traceability of results
- influence of the interpreter on the interpretation results
- presentation of results (such as graphics and text).

Uncertainties relating to the model can be detected by the development of alternative, independent models (see SKI, 1996, Tirén 1996). The question – where are the similarities and differences between the repository site and the surrounding region? – highlights uncertainties in the model.

It is not evident from SR 97 how uncertainties relating to geological and structural geological modelling have been handled.

Is the impact of the investigation on the measurement results taken into account? For example, how do boreholes affect water transport in the rock? How great can this impact be before it results in changes in the natural flow?

9. Summary and Conclusions

The safety of a repository can be summarized by two parameters relating to rock geology:

- isolation
- retardation.

“The rock contributes to isolation by providing a stable chemical and mechanical environment for canisters and the buffer” (A).

Retardation ”means that the time taken for the radionuclide to be transported from the repository to the biosphere is delayed so that hazardous elements can decay considerably before the radionuclides reach man or the environment” (A).

A third – hydrogeological – parameter must be added to those mentioned above, namely, dilution which is not discussed here.

9.1 Isolation

The chemical environment that is important for repository safety is defined by the groundwater chemistry. This topic is not dealt with here.

The function of the bedrock as mechanical protection has been studied from a seismic perspective. Disturbances in the bedrock that are of an order of magnitude that will result in damage to the repository in connection with earthquakes are considered to be improbable.
Only a small share of crustal movements cause earthquakes (see above). The majority of bedrock movements do not take the form of earthquakes. Will a repository be able to withstand these movements and how can one ensure that such movements do not occur at a repository site?

Movements along a fracture plane can have a shear component (movements along the plane) and an extension/compression component (movements/load perpendicular to the plane). Extension opens up structures, thereby increasing their capability to conduct water. How are areas taken into account (classified) that, for instance, have a high frequency of parallel fractures when the orientation of the principal horizontal stress is not well determined and moreover uncertain? A change in the stress direction could imply a change in the hydraulic conductivity of the rock. Could such changes occur in connection with a glaciation? Transport pathways are treated below.

9.2 Transport Pathways - Retardation

Radionuclides can migrate from a repository into the biosphere along planes of weakness in the rock. The transit time depends on the water flow in the rock. The driving force for groundwater transport is mainly gravitation and thereby related to topographical differences in altitude (actually lateral differences in the groundwatersurface). This means that the transport path is determined by the network of fractures and fracture zones in the bedrock and the velocity of the groundwater in the rock is determined by the properties of these structures along with groundwater formation and regional and local topographical differences in altitude. In addition, the hydraulic conductivity of structures usually varies along the length of the structure. Another retardation factor is the sorption of radionuclides to the fracture and pore system of the rock. The extent to which this mechanism occurs is dependent on the type of fracture mineral.

9.3 Late Adaptation to Site-specific Conditions

What does the statement “The KBS-3 system has a flexibility as regards repository depth and layout which allows adaptation to site-specific conditions and to *the information on rock conditions which is continuously collected* during site investigations and repository *excavation* (italics added by author)” made in A (p. 445) mean? How large a deviation from the original model is accepted? How large can the deviations become before SKB has to inform the authorities concerned?

9.4 Basis for Site Selection

One of the purposes of SR 97 is to provide a basis for “specifying the factors that serve as a basis for the selection of areas for site investigations”. However, minor such explicit specifications are provided. Instead it is stated that “these issues are treated and discussed when the site selection programme is discussed”. The reason given for this is that the site investigation programme “includes more than the information sought by the safety assessment” (A page 452).

References

Andersson, J., 1999. SR 97 Data and Data Uncertainties, Compilation of Data and Data Uncertainties for Radionuclide Transport Calculations. SKB Technical Report TR-99-09, Stockholm.

Askling P., 1997. Gideå Lineament Map. An Interpretation Based on Elevation Data Models. SKB PRU-97-06, Stockholm.

G. Bäckblom, G., 1989. Guidlines for use of nomenclature on fractures, fracture zones and other topics. SKB Technical PM 25-89-007, Stockholm.

Lidmar-Bergström, K., 1999. Uplift history revealed by landforms of Scandinavian domes. In Smith. B.J., Whalley, W.B. and Warke, P.A. (Eds), 1999. Erosion, Uplift and Stability: Perspective on Long-term Landscape Development. Geological Society, London, Special Publication, 162, 85-91.

Munier, R., Sandstedt, H., and Niland, L., 1997. Förslag till principiella utformningar av förvar enligt KBS-3 för Aberg, Beberg och Ceberg. SKB R-97-09, Stockholm. (In Swedish).

SKB, 1999a. Deep Repository for Spent Nuclear Fuel. SR 97 – Post-closure Safety. Main Report Volumes I and II. SKB Technical Report TR-99-06, Stockholm.

SKB, 1999b. SR 97 Processes in the Repository Evolution. SKB Technical Report TR-99-07, Stockholm.

SKB, 1999c. SR 97 Waste, Repository Design and Sites. SKB Technical Report TR-99-08, Stockholm.

SKB, 1999d. Djupförvar för lågt- och medelaktivt avfall. Rapport SKB R-99-59, Stockholm. (In Swedish).

SKI, 1996. SKI SITE-94, Deep Repository Performance Assessment Project. Swedish Nuclear Power Inspectorate, SKI Report 96:36, Stockholm.

Slunga, R.S., Norman, P, and Glans, A.C., 1984. Baltic Shield Seismicity, the Result of Regional Network. Geophysical Research Letters 11, 1247-1250.

Tirén, S.A., 1996. Comparison of the SKI, SKB and SKN Geological and Structural Models of the Äspö Area. Swedish Nuclear Power Inspectorate, SKI Report 96:19, Stockholm.

The author

Sven A. Tirén (born in 1947) is a structural geologist educated at Stockholm University and Uppsala University in Sweden (1968-74). He was involved with the Geodynamics Project in the Swedish Caledonides (1970-78), has done prospecting for Swedish mineral resources (1978-1980), and since 1980 has been involved in site characterization of study sites for nuclear waste disposal in Sweden's Fennoscandian shield. He has worked at the Swedish Geological Survey, the Swedish Geological Company, and is currently at GEOSIGMA AB, a geotechnical company in Uppsala, Sweden. His site characterization projects have been both for SKB (Swedish Nuclear Fuel and Waste Management Co.; 1980-1991) and SKI (Swedish Nuclear Power Inspectorate; since 1992).

Comments on SR 97 Chapters 4 and 5 and Supporting Documents

Chin-Fu Tsang

Earth Sciences Division
E. O Lawrence Berkeley National Laboratory
Berkeley, California 94720, USA

SUMMARY

A review was conducted on Chapters 4 and 5 of the SKB SR 97 – Post Closure Safety Main Report, with a background study of Chapters 1-3, as well as a study of the related sections of support documents SKB TR 95-22, SKB TR 99-20 and SKB TR 99-07. Main comments include: (1) Need for Iteration and Integration between Model Conceptualization and Model Investigations; (2) Need for Reviews by Two Types of Experts; (3) Need for Structured Expert Elicitation and Documentation; (4) Need for Careful Definition of Base Scenario; (5) Suggestion of the Use of Zeroth Order Scenario; (6) Confusion in the Definition of "Variables"; (7) Need to Ensure Inclusion of Tertiary and Higher-Order Coupled Processes; (8) Need to Consider Model Abstraction and Associated Uncertainty; (9) Need for Care in Handling Analyses at Different Levels of Details. Additional comments are made more specifically on the THMC diagrams.

SCOPE OF REVIEW

The present review is made for Swedish Nuclear Power Inspectorate (SKI) of the SR 97 - Post-Closure Safety, Main Report (SKB TR-99-06) prepared by Swedish Nuclear Fuel and Waste Management Company (SKB). The review is focused on Chapters 4 and 5 of the SR 97 Main Report, with a background study of Chapters 1-3 of the same report, as well as a study of the support documents SKB TR 95-22, SKB TR 99-20 and SKB TR 99-07 (details of these reports are given in the References).

The main comments, numbered consecutively, are presented below under three headings:

A. Project Coordination and Expert Review
B. Scenarios and Variables
C. Modeling and Analysis

These are followed by a number of more specific comments on THMC Diagrams for the different system elements.

COMMENTS ON PROJECT COORDINATION AND EXPERT REVIEW

(1) Need for Iteration and Integration between Model Conceptualization and Model Investigations

SKB appears to have taken a path of separating (a) model calculations, results and discussion/conclusions, from (b) model conceptualization and model building (i.e., geometry, processes, boundary conditions, and scenarios). Thus the latter is set up by one group of people as a more-or-less independent “data base” of scenarios, features, events and processes, etc; while the former is probably being carried out by another group of people. I am not at all sure that this is a good approach. There needs to be significant communication and iteration between the two parts (a) and (b). To make judgment on (b), e.g., ranking and choice of significant processes, based on one’s intuition and “experience” without the benefit of knowing results of (a) may be a dangerous approach. One need to be on the alert for needed iterations and integration among people in parts (a) and (b) in the safety assessment, especially if the people involved in the two parts are different.

(2) Need for Reviews by Two Types of Experts

Model conceptualization and model building, including geometry, processes, boundary conditions, scenarios, and decisions on process rankings (Section 4.2.4, last paragraph) are certainly an important step. Results of calculations or predictions with the models depend on decisions at this step. If this step is good and correct, the results will be reasonable; and if this step is garbage, the outcome of results and predictions will also be

garbage. In reviewing the supporting document, SKB TR 95-22 and SKB TR 99-20, it appears that the work was done by a limited number of people, mainly within SKB and Kemakta. While these people are very good, they are still limited in their knowledge in terms of the scientific state of art in the multiple disciplines of hydrology, heat transfer, rock mechanics, geochemistry, and microbiology that are involved. I would suggest that their work, especially identification of processes and their rankings, should be seriously (versus superficially) reviewed by experts.

There are two kinds of experts. The first kind is the site-specific or problem-specific experts. These are people that have been studying the site and/or the problem in detail for a number of years. They could be SKB staff and contractors, or people in the waste programs in other countries. The second kind of experts is general scientific experts. These are those in the forefront of their sciences, having a comprehensive knowledge of all related (but may not be apparently relevant) topics in the fields. A proper review needs both types of experts. One also needs to make sure that the experts cover all the scientific disciplines involved. For example, I do not know if the present development of SR 97 Chapters 4 and 5 has made good use of input from recognized scientific experts in the field of microbiology. (Is that the reason paragraphs on this topic are rather brief?) It is also useful to use hand-on scientists in other countries' waste programs to help in the review. Of course all review comments and responses should be properly documented (see next comment).

(3) Need for Structured Expert Elicitation and Documentation

Sometimes appropriate experts may be already involved in the project, but there may be a lack of requesting their input and taking advantage of their experience for particular tasks. Thus the expert review mentioned in the last comment need to be carried out in a structured and documented manner through an expert elicitation procedure. This was done for example in the NIREX95 Program (NIREX95, 1995) and USDOE Yucca Mountain Program (e.g., DOE, 1997). In this way, we can ensure appropriate input by the experts at the right points of the program, with a clear documentation, so that their input can be tracked and future changes followed and understood. There is no evidence in SR 97 that this was done by SKB.

In Section 5.8, the discussions on completeness of system description are too vague. In addition to what is presented here, a well-defined expert elicitation process needs to be done to ensure that the work is at the current state of science internationally.

COMMENTS ON SCENARIOS AND VARIABLES

(4) Need for Careful Definition of Base Scenario

The definition of base scenario and alternative scenarios requires some careful thinking. There can be two views. (a) The base scenario may refer to the scenario for the normal

course of events and alternative scenarios means the cases when something special or unusual happens. Or, (b) the base scenario means that it is the zeroth order, probably neglecting some of the processes present or expected in the future, but it is a case on which the realistic cases can be built. The current definition that the Base Scenario is one in which the present climate persists and no copper canisters have fabrication defects (Section 4.5.2) seems to take the view (b). The real base situation will have climatic change over the next 100,000 years, as the glaciation cycle is of that order, and, further, it is questionable whether the copper canisters can be assumed to have zero defects. This is especially a concern if we consider defects not in the reference of current detection and quality survey capability but in terms of what may show up in the next 100,000 years. We have no such experience, unfortunately. On the other hand, if we take the view of Base Scenario (a), then we should define it as a scenario for the "normal" course of events, which would include glaciation and the presence of a few defect copper canisters.

(5) Suggestion of the Use of Zeroth Order Scenario.

Actually I would rather like the definition of the zeroth order case. Let us define a zeroth order case, not calling it the base scenario, and in this zeroth order case, certain commonly accepted processes are included and documented, such as corrosion, groundwater flow, thermal conduction. Then a number of scenarios can be defined upon it as a basis, and all the THMC diagrams can be defined as deviations or additions to it. This has many advantages over the present scheme. Two most important ones are indicated here. First, in all the process descriptions, we do not have to waste time and effort (and try readers' patience) to present and discuss the obvious processes, because they are already included in the zeroth order case. For instance, I randomly checked SKB TR 95-22 and, without too much effort, found the word "obvious" under the title Motivation on pp. 52, 53, 101, 131 etc. Second, what is even more important is that the current scheme does not focus on potential detrimental factors. Because much effort and writing were spent on well accepted processes, they overshadow detrimental factors, such as heat transfer in the near field buffer by heat pipe effect, heterogeneities, flow channeling, processes in interfaces and gaps, effects of plugs, seals, and rock bolts, etc. These may be either ignored or not in focus. And it is these detrimental effects that may have an important impact on safety.

(6) Confusion in the Definition of "Variables"

The definition of "variables" for the THMC diagrams leaves much to be desired. As it is now, it means not only variables, but also geometric factors, current or initial conditions, as well as boundary conditions. It also seems to include items that are more like processes, such as "groundwater flow". At a minimum, the list of "variables" should be listed in a sequence such that these different types are in successive groups and not all mixed up. Also the variables tend to indicate standard parameters and sometimes overlook parameters that control potential detrimental factors such as flow channeling, tracer fast paths, and gaps and interfaces. A greater effort to build into the scheme a focus on detrimental factors will be very critical for safety assessment.

From Section 4.2.5 and Section 4.2.6, it seems that processes are coupled with each other only through "variables", and my first reaction is that there may be no coupled processes in this approach. However on later readings, I think that there are indeed coupled processes included, but in a curious way through the "variables". Then the definition of variables becomes strange by necessity. Thus one finds that "groundwater flow" appears both as a variable and as a process in the THMC diagrams. It is also strange that "permeability" which is a key parameter in all site characterization programs in many countries is not included in the list of variables. I assume that it is hidden in the variable "groundwater flow".

Considering repository geometry and boundary as "variables" (Section 4.2.6, last sentence) is also an unusual approach. I would suggest that one defines the geometry and boundary within the zeroth order framework (see Comment (5) above) and then call the deviations or changes, due to, for instance, excavation or heating, as variables.

(7) Need to Ensure Inclusion of Tertiary and Higher-Order Coupled Processes

The processes shown in the THMC diagrams are binary, i.e., how variable A affects process B and vice versa, since they are based on two-dimensional interaction matrices. Are there tertiary-coupled processes? I suspect the binary processes discussed in SR 97 do indeed include tertiary and higher ordered ones in the sense that in the binary considerations, all the conditions for the third or more other process are considered. In this sense this binary approach is acceptable. But still care needs to be exercised to ensure no important higher-order coupling is overlooked.

COMMENTS ON MODEL AND ANALYSIS

(8) Need to Consider Model Abstraction and Associated Uncertainty

In Table 4-1, four steps of analysis are indicated, which are fine and commonly accepted. However some countries have recognized a need to divide the "analysis" or modeling step into two. One is a kind of detailed model, trying to model and understand in-situ experiments and relevant data, reproducing them within an accepted degree of uncertainty. Often this model has to account for very special test conditions, such as strongly convergent flow, wellbore skin effects, etc., and are too complex to use in safety assessment of a potential repository. Thus there is a need for a simplified or abstracted model that can be used in multiple Monte Carlo simulations for probabilistic predictions for the many scenarios. Associated with model abstraction are the abstraction uncertainties, which needs to be considered. SR 97 appears not to have recognized this need.

(9) Need of Care in Handling Analyses at Different Levels of Details

In Section 4.5.1, it is stated here that the methods for and the depth of analysis vary widely between the different scenarios. This is understandable, but care needs to be taken in evaluating the results (Tsang, et al., 1994), especially when one is weighing together all the results of the different scenarios (see third paragraph of Section 4.4.2). Often, a shallow analysis shows less detrimental factors to safety than a deeper analysis.

SPECIFIC COMMENTS ON THMC DIAGRAMS

A. Fuel/cavity (Sections 5.3.1-5.3.3)

(1) Among the variables for geometry, it may be useful to point out the need to consider gaps and interfaces as well as cavities. These are discussed in SKB TR 99-07 Processes Report, p. 15. Perhaps the term cavity in SR 97 includes these types of cracks. It may be useful to clearly state so. Also, instead of water composition, one may want to use "hydrochemical environment" to focus more on fuel-chemical interactions.

(2) For the process, Heat Transport, I do not understand the stated dependence on material composition. The SKB TR 99-07 Processes Report (p. 25) does not justify this. I suspect that it was included because of the thermal conductivity being dependent on material composition. But I think that thermal conductivity can be included as one of the variables (why not?) It is quite a stable parameter, not so sensitive to the detailed material composition. This is just like we do not characterize heat transfer as dependent on the vibrational characteristics of electrons and atoms in the material.

(3) I am surprised that Thermal expansion/Cladding failure is not related to Temperature and Material composition. I would think that temperature causes thermal expansion and material composition is related to expansivity of materials (there is no variable called Material expansivity). On the other hand, its dependence on "Hydrovariables" is probably not so important. The Processes Report (SKB TR 99-07, pp. 29-30) does not explain these points.

(4) How about the processes of thermal cracking, cavity formation and cavity shape changes? These are not in the diagram.

B. Copper canister/Cast iron insert (Sections 5.4.1-5.4.3)

(1) I believe that here crack formation, gaps and interfaces are important issues. They are probably included in this section in some fashion, but it would be much better if they are brought out in a more highlighted way among the list of variables or in the form of processes in such cracks and cavities.

(2) I am surprised that hydrogeochemical environment is not among the variables as they are obviously related to potential corrosion.

(3) There is no indication of concern related to microbiology, which may be potential promoters of corrosion or other effects. Is this correct?

(4) It is surprising that the deformation of copper canister and iron insert is independent of temperature. It may not be reasonable to separate out the process of thermal expansion from deformation. Also in the Processes Report (SKB TR 99-07, p. 63), it is clearly indicated that the creep phenomenon depends on temperature.

C. Buffer/Backfill (Sections 5.5.1-5.5.3)

(1) The list of variables seems to focus on routine items and misses important issues, such as heterogeneities, gaps and interfaces, colloidal and microbiological factors.

(2) Among the variables, what is "Pore Geometry" referring to? Does it refer to porosity (then use porosity as a variable; why not?), or does it refer to the shape of the pores? If it is the latter, I do not see why it should affect water and gas transport or thermal expansion to any significant extent.

(3) Also among the variables is the impurity content, which for backfill is the crushed rock, comprising 85% of the backfill material. It really should not be called impurity, since it is the bulk of the material intentionally designed this way.

(4) Also among the variables, what is the difference between smectite content and smectite composition? The definitions in Table 5.3 and in the Processes Report (SKB TR 99-07, p. 92-93) do not seem to give a clear distinction. Perhaps there is a difference, but such details may not be needed in the Diagram where the other variables are treated in such a gross way (for example, the use of the term hydrovariables to include all hydrological factors).

(5) It may be useful to subdivide Heat Transport into separate items, such as conduction, convection and heat pipe process. They are treated quite differently in terms of mathematical calculations and functional dependence. The heat pipe effect may be important where there are two phases present. Vapor would move in the pores, much more effectively than water, and then condenses in the cooler part, resulting in a very effective heat transfer mechanism. Such effect would occur even below water boiling temperature. This process is implied in the discussion on p. 98 of the Processes Report, but is not highlighted as an effective heat transfer process.

(6) In the processes involving water and gas, it may be useful to include evaporation and condensation, as there will be a significant temperature gradient across the buffer. This is mentioned in the comprehensive discussion of the hydrological processes in the buffer on pp. 102-107 of the Processes Report (SKB TR 99-07), but many of the key issues discussed there are not reflected in the THMC Diagram. In contrast, much more details on "Solutes" and "Radionucludes" are shown in the Diagram.

D. Geosphere (Sections 5.6.1-5.6.3)

(1) Among the variables is the item, Engineering and stray materials, which is defined in terms of chemical composition and quantities of grouts, rock supports and plug, etc. I think what is also very important are the hydraulic effects of these seals and plugs, and whether they will introduce additional flow paths connecting major fractures or fracture zones. For example, rock bolts may corrode with time and form flow paths. They can be several meters long, and that is comparable to fracture spacing near the drift and is very probably longer than the local fracture spacing if there is a significant disturbed zone there.

(2) The heat pipe effect discussed above will also happen in the geosphere near the repository, where there is a significant temperature gradient. This should be included.

(3) Among the processes in the THMC Diagram, the thermal transport would give rise to temperature gradients, which will in turn induces groundwater pressures. I believe that there should be an arrow to it. The dependence of thermal transfer on Fracture geometry, Rock stress and Fracture minerals should not be significant, in contrast to what are indicated in the Diagram. This is confirmed by the discussion in the Processes Report (p. 175). Also, the dependence on the specifics of Matrix minerals should also not be important. It is more related to thermal conductivity (why not call that a variable?) As indicated on p. 175 of the Processes Report, thermal conductivity is very stable with respect to variations in the matrix mineral composition. The variation among Swedish and Finnish rocks is only between 2.7 to 3.6 W/(m.K), which is a very narrow range compared to variations in many other chemical and hydrological factors.

(4) Concerning advection and mixing, Section 5.6.3 (middle of page on p. 72) mentions "mixing of different types of water from different parts of the geosphere". This statement needs to be taken with great care. The usual concept of mixing because of dispersion (defined with a dispersivity length) can be very misleading or even wrong. Such a theory is only valid if the measurement or sampling scale is equal or larger than the dispersivity (Tsang, 2000). If the sample scale is smaller, mixing is only due to diffusion, which is a much smaller effect.

(5) Concerning the microbial process in the THMC diagram, I am surprised that it does not depend on groundwater and gas flow, because sustained microbial action requires the availability of nutrients, which are carried by groundwater and gas flows.

REFERENCES

DOE. *Civilian Radioactive Waste Management System Management and Operating Contractor: Saturated Zone Flow and Transport Expert Elicitation Project,* prepared by Geomatrix Consultants, Inc., San Francisco, California and TRW, Las Vegas, Nevada, WBW 1.2.5.7, October 1997.

NIREX95. *A Preliminary Analysis of the Groundwater Pathway for a Deep Repository at Sellafield. Volume I: Development of the Hydrogeological Conceptual Model. Volume II: Derivation of Effective Hydrogeological Parameters for Regional Modeling. Volume III: Calculations of Risk.* United Kingdom NIREX Limited, Science Report 5/95/012, 1995.

SKB TR-95-22. Technical Report. *The Use of Interaction Matrices for Identification, Structuring and Ranking of FEPs in a Repository System: Application on the Far-Field of a Deep Geological Repository for Spent Fuel*. K. Skagius, A. Ström, and M. Wiborgh, Swedish Nuclear Fuel and Waste Management Co., Stockholm, Sweden, November 1995.

SKB TR-99-06. Technical Report. *Deep Repository for Spent Nuclear Fuel, SR 97 – Post-Closure Safety, Main Report Summary*. Swedish Nuclear Fuel and Waste Management Co., Stockholm, Sweden, November 1999.

SKB TR-99-06. Technical Report. *Deep Repository for Spent Nuclear Fuel, SR 97 – Post-Closure Safety, Main Report Volume I.* Swedish Nuclear Fuel and Waste Management Co., Stockholm, Sweden, November 1999.

SKB TR-99-06. Technical Report. *Deep Repository for Spent Nuclear Fuel, SR 97 – Post-Closure Safety, Main Report Volume II.* Swedish Nuclear Fuel and Waste Management Co., Stockholm, Sweden, November 1999.

SKB TR-99-07. Technical Report. *SR 97, Processes in the Repository Evolution, Background Report to SR 97.* Swedish Nuclear Fuel and Waste Management Co., Stockholm, Sweden, November 1999.

SKB TR-99-20. *Technical Report. SR 97 – Identification and Structuring of Process*. K. Pers, K. Skagius, S. Södergren, M. Wiborgh, A. Hedin, L. Morén, P. Sellin, A. Ström, R. Pusch, and J. Bruno, Swedish Nuclear Fuel and Waste Management Co., Stockholm, Sweden, December 1999.

Tsang, C.F., L. Gelhar, G. de Marsily, and J. Andersson, *Solute Transport in Heterogeneous Media: A Discussion of Technical Issues Coupling Site Characterization and Predictive Assessment.* Advances in Water Resources, Vol. 17, No. 4, pp. 259–264, 1994.

Tsang, C.F., *Modeling Groundwater Flow and Mass Transport in Heterogeneous Media– Issues and Challenges,* invited Keynote Paper, Proceedings of the International Association of Hydrogeologists XXX Congress 2000, Capetown, South Africa, 26 November –1 December, 2000. A. A. Balkema Publishers, Rotterdam, the Netherlands.

APPENDIX

Dr. Chin-Fu Tsang is a Senior Staff Scientist in the Earth Sciences Division and Head of the Department of Hydrogeology and Reservoir Dynamics at the Ernest Orlando Lawrence Berkeley National Laboratory. His research ranges from geothermal reservoir dynamics; thermohydraulic processes for underground thermal energy storage; dynamic borehole fluid logging methods, to coupled thermo-hydro-mechanical (THM) processes in fractured rocks, and numerical stochastic modeling of flow and transport in strongly heterogeneous systems. Under the last topic, his research emphasis has been on channelized or preferential flow in both saturated and unsaturated media. Dr. Tsang has published extensively in his field. He has over 300 scientific reports and invited or keynote presentations, including more than 100 papers in refereed journals. He is a co-author of the popular Water Resources Monograph 10, *Groundwater Transport*, published by the American Geophysical Union (AGU) in 1984, which is now in its fifth printing. He co-edited six other books in such areas as flow and contaminant transport in fractured rocks, deep well injection, and coupled thermo-hydro-mechanical processes. He was the Guest Editor of special issues of *International Journal of Rock Mechanics and Mining Sciences, Environmental Geology,* and *Hydrological Science and Technology*. Dr. Tsang has also been active in international research cooperation. He played a key role in such international cooperative research projects as HYDROCOIN and INTRAVAL. He is currently the Chair of Steering Committee for the International DECOVALEX project on coupled THM processes.

Review of SR 97

Clifford I. Voss

U.S.Geological Survey
Water Resources Division
432 National Center
Reston, Virginia 22092, USA

This review is an independent technical evaluation of SR 97 by C.I. Voss. It was carried out in response to a request of SKI as a part of ongoing technical and research cooperation between USGS and SKI.
*This review is **not** an official USGS statement on SR 97 or on any of the topics mentioned herein.*

Summary

The safety analysis conducted by SKB for SR 97 is impressive in terms of both scale and content. In addition to an eventual solution to Sweden's nuclear waste isolation question, much general scientific knowledge of real value in other applications will be created as a by-product of SKB's efforts. This review focuses on those geoscience aspects of SR 97 that have the most important effects on radionuclide release from each barrier. Indeed, SR 97 elucidates the most important geoscience parameters that control releases from the near field and the far field; these comprise mainly the transport resistance parameter, and the sorption coefficients for each nuclide, the matrix diffusion coefficient, and the Darcy flux.

The Main Report is the most important document in SR 97 inasmuch as it is the only one that brings together all of the supporting work to answer the question of safety. Unfortunately pervading the good supporting work done is the impression that the Main Report is not balanced, that it emphasizes optimistic aspects and downplays the negative.

SKB specifies 3 main requirements to guarantee proper repository function: a non-oxidizing subsurface environment, temperatures less than 100 C, and a mechanically stable low-permeability buffer surrounding the canisters. The first and third requirements are not thoroughly proven by SKB. One source of near-field doubt stems from the consequences of combinations of scenarios in which several negative events are linked, while the effect of each scenario is mainly evaluated only independently in SR 97. More pertinently, disastrous breakdown of complex systems may occur due to a chain of linked failures. For example, in the glacial scenario: high ground-water flow (possible ablation of buffer and high fluid transport), change in ground-water chemistry (even the possibility of oxidizing conditions), new flow paths, significant changes in mechanical stress and possible motion along faults (which may also generate new flow paths), and so on, are likely to all occur together.

Despite incomplete proof of the required conditions, SR 97 concludes that the engineered barriers in the near field will certainly isolate radionuclides to levels well below Sweden's regulatory limits. A by-product of SKB's optimism about the near field is that other barrier functions were never fully tested in SR 97, limiting the completeness of the analysis.

SR 97 Main Report results lead to the conclusion that all possible repository sites are equally serviceable due to the excellent near field barriers. Although SKB has only a few potential sites available at present, (and these are available only because of local political

acceptance, not because these sites have the best conditions in Sweden for a repository) it seems obvious that SKB management would wish to downplay differences among sites. This would become harmful to progress toward repository siting should it result in acrimonious public discussion. On the other hand, site characteristics that would improve a repository's safety margin are directly motivated by specific SR 97 supporting documents, including low-conductivity rock mass, easily-characterized spatial properties, and location in a first-order recharge area (giving very long flow paths from the repository and thus greater isolation of radionuclides). However, SKB never drew siting preference conclusions, maybe because this would limit choices to sites that are not politically popular.

Specifically in regard to the hydrogeologic analysis, SR 97 shows the sites to be complex possibly to the extent that they can never be sufficiently characterized. To deal with this problem, the ground-water modeling done in SR 97 employed the popular approach of generating hydrogeologic variability using arbitrary probability distributions for parameters. This approach disguises lack of knowledge about a site in something that appears to be detailed and complex. Despite the convenience for analysts who are asked to generate fluxes, travel paths and travel times, it is dangerous to use unproven probability distributions as the basis for assessment of hydrogeologic impact on repository safety. There may be serious doubt that the fluxes and path values derived from SR 97 ground-water modeling are appropriate for determining near-field release and far-field transport because they are based on poorly founded probabilistic assumptions, on weak hydrogeologic structural models of the sites, and on static boundary conditions, despite the expectation of strong climate change effects. In this light, it is interesting that SR 97 directly used very little of the extensive ground-water modeling results, funneling all of the considerations and complexities for each site into a few selected values for use in release, transport, and dose calculations. It can be argued that, if these few values are all that are needed for performance assessment, *they can be equally well determined by simple hydrogeologic scoping calculations for a site, rather than through the type of extensive effort applied in SR 97.*

This reviewer

Dr. Clifford I. Voss is a senior scientist in the National Research Program of the U.S. Geological Survey and Chief of the research project "Subsurface Transport Phenomena". He is the Executive Editor of *Hydrogeology Journal,* official journal of the International Association of Hydrogeologists. His expertise pertinent to the present review is in characterization and quantitative analysis of hydrogeology at various spatial scales in field sites, development of quantitative methods and simulation models for analysis of subsurface hydrology, and evaluation of variable-density subsurface fluid flow with solute and energy transport. Dr. Voss lectures and teaches courses in these subjects. Dr. Voss has also worked on ground-water systems in Sweden since 1978, initially at KTH (Royal Institute of Technology) and VBB AB, and has worked extensively on hydrogeologic aspects of nuclear waste issues in Sweden with SKB, Geosigma AB (formerly SGAB, Swedish Geological Co), and particularly with SKI since 1989.

As a specialist in quantitative hydrology, in the physics of subsurface fluid flow and transport of energy and solutes, as well as in hydrogeology, this reviewer has concentrated on aspects of SR 97 related to these subject areas. Indeed, key questions of ultimate repository safety depend on the functioning of the geologic barrier as part of a multi-barrier safety system, so these are topics of importance.

Introduction

The analysis conducted by SKB for SR 97 is impressive in terms of both scale and content. The large amount of effort expended on this project shows clearly in its excellent quality. This reviewer finds the SR 97 work to be among the best organized SKB projects to date with significant technical depth in most of the highly varied scientific and engineering aspects that need to be combined to carry out Performance Assessment (PA) for the SFL2 high-level nuclear waste repository. This reviewer congratulates SKB for managing to bring together many years of world-class detailed hydrogeologic field data collection, and engineered barrier development, in a new analysis intended to answer the direct question of long-term repository safety. In addition to an eventual solution to Sweden's nuclear waste isolation question, much general scientific knowledge of real value in other applications will be created as a by-product of SKB's efforts.

Approach to the review

In an analysis of this great scope, there is obviously much to appreciate and discuss, as well as to criticize. My approach, in view of a limited time available to conduct the review, is to consider those geoscience aspects of SR 97 that have the most important effects on radionuclide release from each barrier; these are the aspects that ultimately control the dose. This approach requires that the controlling geoscience factors on release, transport and dose be identified. For the factors defined by process parameters, both the parameter values and the assumptions made in selecting these values are

reviewed. Factors that are related to events are considered separately. Because only a very small fraction of all results of the extensive and varied analyses provided in the supporting reports was finally used to determine dose consequences, the stated review approach greatly simplifies the task, and simultaneously focuses on the critical aspects.

One positive result of SR 97 is that it elucidates the most important geoscience parameters that control release from the near field and the far field. The primary control describing sorption and matrix diffusion in the far field is the transport resistance parameter, F. This parameter depends upon the surface area of fractures in the rock, a_r, the Darcy flux, q, and the transport reach, L. Of secondary importance are the sorption coefficients for each nuclide, K_d, and the matrix diffusion coefficient, D_e. The hydrogeologic parameter that most controls near-field release is again the Darcy flux, q. The central importance of these parameters and focus on them has been developing over some years prior to SR 97 because of both SKB and SKI work. SR 97 confirms their strong influence on repository safety. SR 97 identified the other important factor that controls dose, the biosphere, which was reviewed only in a general sense.

The SR 97 – related reports that were referred to or specifically reviewed in whole or in part are:
SKB TR 97-01 09 20 21
SKB TR 98-23 24 60
SKB TR 99-02 06 07 08 09 13 18
SKB R 99-38 39

General Observations

Before discussing specific technical aspects, some general observations are in order. The Main Report is the most important document in SR 97 inasmuch as it is the only one that brings together all of the supporting work to answer the question of safety. An impression of the Main Report that unfortunately pervades the good supporting work done is that it is not balanced, that it emphasizes optimistic aspects and downplays the negative.

SKB specifies that there are three main requirements that will guarantee proper function of the copper-canister-type SFL2 repository, providing extended radionuclide isolation capacity:

- A non-oxidizing subsurface environment
- Temperatures less than 100 C
- A mechanically stable low-permeability buffer surrounding the canisters

To date, it seems that the first and third requirements have not been thoroughly proven by SKB. There are significant discussions ongoing concerning the possibility of extended periods of oxygenated ground waters invading the repository in association with future periods of sub-glacial melting. Only minor effort has been expended in evaluating this important possibility within SR 97. Further, there are still questions surrounding the long-

term stability of the bentonite. Circumventing these concerns, the general conclusion of SR 97 is that the required conditions will exist for the repository and that the engineered barriers in the near field will certainly isolate radionuclides to levels well below Sweden's regulatory limits.
Following in-depth review of SR 97 this reviewer finds two ways to interpret this primary positive conclusion of the SR 97 Main Report:

1- If the conclusions of the Main Report are to be taken at face value then the repository truly works as shown with almost perfect near-field function. In addition,
    a. the geosphere will serve little to contain radionuclides because near field barriers contain the waste without problem, and
    b. there is no practical difference in safety among sites (at least sites as varied as A-, Be-, and Ce-berg) because the near field functions perfectly at *any* site. The impression is given that if the repository were placed underground almost anywhere in Sweden, it would function in this safe manner.

2- If one were to be more skeptical of the conclusions drawn in the Main Report, then it could be considered partly as a public relations document intended to convince readers that irrespective of location, the repository is safe due to the engineered barriers. Indeed, it is SKB's mission to create such a repository, and though there exists more pessimism in many of the supporting reports with regard to various barrier functions, SKB has only brought forward a generally positive assessment in the Main Report.

It is difficult to believe in a nearly perfect near field. This reviewer is skeptical about the stability of canisters and that only 1-5 holes might exist in or develop in 4000 canisters within 100s of ka. This is only speculation, however, as this reviewer does not profess expertise regarding canister construction or evolution. In any case, according to SKB, the canister is the main barrier that controls release.

A negative result of SKB's optimism about the near field in SR 97 is that the function of the other barriers was never fully tested. The approach used in SR 97 makes it difficult to evaluate the function of the other barriers in the multibarrier system, as they are not given a chance to act as the prime barrier in the analysis. It would be expected that SKB consider thorough analysis of scenarios where more canisters are breached (and earlier), with the specific intent of evaluating the function of the other barriers more fairly, fully and independently. This would not be an admission by SKB that the near field is not reliable, but rather a means of building confidence in the multibarrier system.

Another aspect of SR 97 Main Report results that is difficult to believe is that all possible sites are equally serviceable. One can understand why it would be advantageous to SKB if location did not matter. SKB has only a few potential sites available at present, and these are available only because of local political acceptance, not because these sites have the best conditions in Sweden for a repository. While this situation is not a valid reason to

downplay differences among sites, it seems obvious to ascribe such a motivation to SKB management, and this could become harmful to progress toward repository siting should it result in acrimonious public discussion.

Instead, it would seem to be in SKB's interest to seek out geoscience differences in sites that would *improve* a repository's safety margin. Some obvious positive hydrogeologic characteristics would be, for example, a low-conductivity (infrequently fractured) rock mass, spatial properties that can be well characterized (relatively simple), and location in a first-order recharge area (giving very long flow paths from the repository and thus greater isolation of radionuclides). Indeed these particular characteristics are directly motivated by specific SR 97 results in supporting documents, but SKB never drew siting preference conclusions, maybe because this would limit choices to sites which are not politically popular.

Data Report

To critically review the quantitative results obtained by SKB, the input parameters to the transport and dose calculations must be carefully evaluated. This can be done almost completely by reviewing only Andersson's Data Report (TR-99-09). This is arguably the key report in the entire SR 97 analysis. Values for every aspect of the all-important radionuclide transport and dose calculations are selected here. Andersson has in fact done a most careful critical review of all SR 97 work leading to and prior to the dose calculations. His analysis and comments are rather well considered, objective and fair when judgment is called for. TR-99-09, in a sense, may be the best critical review available of all of the supporting work that went into SR 97. Indeed, many of the criticisms made in the present review by this reviewer were also found, clearly stated, in the Data Report.

However, SKB did not carefully interpret and apply Andersson's considered comments and choice of parameters. For example, Andersson points out a number of times that the median value of Darcy flux, q, selected to represent the 'Reasonable' case, is only an "illustration", and is not the most likely or 'normal' case at each site. This important distinction does not appear clearly in the SR 97 Main Report and this lack could be interpreted as part of SKB's selective reporting of mainly positive results. Although the implications of 'Pessimistic' values are also quite visibly reported in the Main Report, the reader is given the impression that these cases are extreme and rather unlikely. In reality, the 'Reasonable' case is not necessarily likely either.

Near field

For the near field flow, the 'Pessimistic' case value selected, that the flow is 5 times the darcy flux, $q_1=5q_0$, is quite arbitrary and the sensitivity of releases to this should be evaluated.

A possibly important factor not considered is that the EDZ (excavation disturbed zone) may not only increase conductivity in the tunnel bottom, but also may connect every single deposition hole to the most transmissive structure that intersects the drift. This could increase the importance of the EDZ discharge path in the near field to all canisters and give larger fluxes to each.

The F parameter

Because the primary control on radionuclide migration through the far field is the F parameter, it is of greatest importance to evaluate this as carefully as possible. The SR 97 method selects F values using a_r primarily based on conductive fracture frequency in borehole hydraulic tests with packers. This approach may result in a significant overestimate of area available for sorption and matrix diffusion of radionuclides because of the following:

- The entire fracture surface is not available for sorption. Likely, only a portion of the fracture surface is available for sorption. Geometric evaluation of the available surface was done by Dverstorp and others (SKI 96:14) demonstrating a range of possible values for Aberg including values much less than the total planar surface.
- Not all fractures participate equally in sorption as those with greater transmissivity and connectivity conduct higher water flux and make up the 'trunk' of the percolating net of flow channels. Leaks from canisters would tend to 'seek out' these preferred pathways (after flowing through a few *tributary* fractures) and would be subject to sorption mainly in the 'trunk'. Thus, the effective area potentially available to escaping radionuclides can be significantly less than the mean a_r for the entire rock.
    - The most conductive fracture segments tend to accumulate flows from other less-conductive fractures and their surface area plays a larger role in F than the conductive tributary fractures. Considering that all conductive fracture segments contribute equally to the F of the rock would thus lead to a significant overestimate of F. *In a sense, this could be explained by describing a spatial correlation between q and a_r.* SR 97 assumes that these parameters are minimally correlated, for the practical purposes of the analysis.
    - Andersson (TR-99-09) realizes this and argues that because the 'conductive fracture frequency technique' used underestimates a_r, this underestimation somehow offsets the lowering of a_r that would result when considering spatial correlation of q and a_r. However, this is purely conjecture, as the magnitude of lowering due to the spatial correlation is unknown, and it may be much more significant than that of the technique-based underestimate.
- Indeed, from geometric considerations alone, and without considering a further decrease due to spatial correlation of q and a_r, Dverstorp and others (SKI 96:14) find much lower possible values for Aberg (F values about 100 times lower than the Pessimistic values used in SR 97).

In summary, the lower F values selected as 'Pessimistic' values are not necessarily near the lower end of the range of feasible or even reasonable values. For the 1D far-field transport analysis, an effective value of area, a_r, should be used that accounts both for possible reduction of available surface due to internal geometry of percolating fractures, and due to the concentration of flow in the most transmissive and well-connected fracture segments. These considerations could also significantly lower, by some orders of magnitude, what would be expected as 'Reasonable' values. This would have a large impact increasing all far-field releases and dose.

Other parameters

According to SKB, the maximum penetration depth for matrix diffusion, another parameter affecting far-field transport, affects far-field release of mainly non-sorbing nuclides. However, SKB has selected the maximum possible theoretical value of this parameter for each site, half the distance between fractures, 2m to 20m. Research in other countries shows that matrix diffusion is limited to a narrow band of rock (on the order of centimeters thick) adjoining the flowing fractures. Lower values than those selected by SKB would tend to increase the maximum release from the far field and cause it to travel more swiftly along the flow path. Thus, SKB's selection of values of this parameter for PA is not conservative, and it affects a few of the nuclides important to dose.

K_d is the linear sorption coefficient that has different values for each radionuclide and that takes on different values depending on both water chemistry and rock composition (i.e. which minerals coat fractures). SKB considered only minor variation of this parameter based on whether water types would be fresh or saline. However, the SFL2 repository and discharge paths at each site may encounter waters that are fresh (rainfall or glacial meltwater), seawater, or shield brine. Migration of subsurface water bodies during climate change was not carefully considered by SKB, and the variations of K_d are thus incomplete. Further, K_d depends on rock type and on the coatings in flowing fractures and K_d variation based on these factors was not considered at all in the PA. It is not clear what effect such variations would have on ultimate dose.

Effective diffusivity is another important parameter that controls the retardation of radionuclides in the far field. Values for each radionuclide were selected by SKB irrespective of site. The values were determined based on a limited number of laboratory diffusion experiments using small rock segments and an interpretive method to apply these results for the determination of other nuclides. There is some uncertainty concerning diffusivity values determined in the laboratory due to insufficient sampling of heterogeneous pore distributions in the rock when using only a few samples, and due to unloading of the rock during testing. Both of these factors may tend to over-estimate the diffusivity, providing an optimistic PA. Future in-situ measurements by SKB may be able to verify these values, but these must be treated with caution at present. To accommodate this uncertainty, SKB should have employed a range of diffusivity values for each nuclide.

Site characterization

Aberg was most recently and most intensely studied of the three sites. Thus, the local hydrogeologic characterization has the highest resolution of the three, although the area characterized is small. There are still significant uncertainties and unknowns inherent in SKB's hydrogeological structural model of the site, which only covers the region immediately surrounding the Hard Rock Laboratory on the southernmost tip of the island. The Aberg repository is much wider than the primary area in which most field data exists, and thus the better-defined part of the structural model provides little support for the analysis. Little structural detail is known for the primary portions of the repository in the northern part of the island and below the straight.

Beberg was investigated in the mid to late 1980s and most efforts were directed at understanding the hydrogeology associated with and the flow through and around a single highly conductive fracture zone (Zone 2) of limited lateral extent. Near Zone 2, and to the depth of Zone 2, the site characterization gave relatively high resolution of hydrogeologic features. Outside of this immediate area, resolution was much lower. The effect of Zone 2 stands out in model results apparently indicating the importance of this one structure as a control on ground-water flow and movement of salt water. While a naive view may accept that this is the only such structure in the entire Beberg area, it is unlikely that the investigation program luckily intersected the only one that exists in the area. Rather, the modeling shows how careful field characterization near Zone 2 has demonstrated an under-characterization in the rest of the area. Other similar highly conductive fracture zones and segments are possible. SKB should have considered the potential impact on safety in more significant variants with similar conductive structures at various depths and locations throughout the area.

Ceberg is the oldest site of the three. Ceberg is unusual among SKB's study sites in the sense that it is difficult to distinguish the transmissivity of the rock mass and fracture zones at the site. Fracture zones seem not much more permeable than the rock mass, as fracture zone and rock mass conductivity have similarly large variation. However, this judgment is based on an early SKB field characterization program; investigations took place there nearly 20 years ago. While there are some geologic arguments for uniformity of transmissivity at Ceberg, it is not impossible that a return investigation of the site with a larger number of boreholes, better resolution, and current approaches would resolve fracture zones that are significantly more conductive than the rock mass. The old data may indicate simply that the site was not sufficiently characterized to resolve structures. SKB should have significant interest in finding out whether the site is as un-fractured and of such low conductivity as the old data indicates. If true, this could mean that a site exists which has some clear hydrogeologic advantages for improving the repository's safety margins. At present, there is some doubt that the SR 97 evaluations for Ceberg are at all meaningful.

Ground-water modeling

The HYDRASTAR stochastic continuum approach is used in SR 97 to generate fluxes and flow paths. This approach assumes forms of upscaling and of the spatial conductivity that have been used in other stochastic continuum studies, but have no real basis in fractured rock theory or in data wherein variability is so great. The types of spatial distributions and spatial correlations assumed are completely arbitrary. Use of such spatial probabilities probably gives the wrong connectivity and percolation through the rock, with the following results:

- Selection of median and 95% parameter values of flux and travel time from distributions resulting from model runs is arbitrary.
- The direct use of the entire distributions for probabilistic PA is not meaningful.

Though this approach is often suggested when deterministic data are lacking, generating variability with an arbitrary probabilistic distribution is a way of disguising a lack of knowledge about a site in something that appears to be detailed and complex. The appeal of this approach is that it is a type of sophisticated extrapolation that fills in values where no data is available. The spread of results may cover the true range (or may not) and there is no scientific proof that results are correct or meaningful. While convenient, *it seems dangerous to use this as the primary means of assessing hydrogeologic impact on repository safety through generation of fluxes travel paths and travel times.*

In an attempt to account for this type of arbitrariness in the underlying assumptions of any given model, SKB used a variety of ground-water model types on Aberg. However, the primary outcome of this large modeling effort was mainly a comparison of flux distributions. The reported result is that the HYDRASTAR model assumptions give as wide or wider variability as any other model; thus, HYDRASTAR is 'good enough' to use for the PA (performance assessment). This reviewer agrees that it may be good enough in the case where use of a model for PA is a statutory requirement, but feels that the same result could have been obtained without use of the ground-water models at all – but with basic scoping calculations.

> In defense of ground-water modeling (both deterministic and stochastic), this will most certainly be done for the real future PA, but it should be only as an exercise and demonstration that the data, when put in the context of the model's ground-water physics, are not inconsistent with our intuitive understanding of flow at a site. Results of such modeling cannot be proven and numerical modeling is best used for building scientific intuition into flow phenomena in fractured rocks, not for making predictions.

Additionally, hydrogeologic structural variants, discretization and parameterization variants were compared with all of the models for Aberg and with a 'base model' for Beberg and Ceberg. The result, that the spatial variability for each site has greater impact on the flow field than the different variants, and that use of HYDRASTAR is 'good enough', can be questioned from an additional point of view. It is likely that the variants

were not ‘variant enough’ to cover the range of reasonable possibilities at such heterogeneous sites. Thus, despite the SR 97 conclusion, there clearly remains a question of whether spatial variability and uncertainty is the only factor, or even the main factor, that needs to be considered when carrying out PA.

Further to the above discussion, there is no real purpose in carrying out careful in-depth review of the extensive ground-water modeling efforts made for SR 97. SKB has directly used *very little* of the modeling results of these efforts, funneling all of the considerations and complexities for each site into very few selected values for use in release, transport, and dose calculations. It can be argued that, if these few values are all that is needed for PA, *they can be equally well determined by simple hydrogeologic scoping calculations for a site.* An opposing argument (though not believed by this reviewer) is that the modeling results were not used extensively enough in the sense that the real limitation to the PA is the overly simplistic type of transport model used in the near and far fields (e.g. 1D with constant parameters) which can accept only a few of the underlying model results.

Indeed, little was learned from ground water modeling insofar as the PA is concerned, other than flux, q_0, and flow paths (length, outlet points, and travel time).

- Flux, q_0, can be directly obtained from a simple evaluation of site hydrogeology, and a range may be obtained from simple evaluation of heterogeneities and uncertainty.
- Flow path is one of the weakest results of the ground-water modeling as it depends strongly on the assumed boundary conditions, model domains, and very poorly known hydrogeologic structure.
- Boundary conditions change with time (e.g. due to climate changes) making flow path results of the SR 97 models with static boundary conditions even more unreliable.
    - Particularly, outflow points may shift dramatically to other points within or even external to the modeled regions, calling into question any biosphere analysis that is done only on the basis of discharge points from such ground-water modeling.

In summary, this reviewer has serious doubt that the fluxes and path values derived from the ground-water modeling are the appropriate ones to use when determining near-field release and far-field transport. They are based on a set of poorly founded probabilistic assumptions, on weak hydrogeologic structural models of the sites, and on static boundary conditions despite the expectation of strong climate change effects. It may be more meaningful to carry out simple scoping analyses that deal directly with the range of possibilities and conditions that are intuitively expected for a given site. Given the poor state of knowledge of variability in fractured rocks, models should rather be used in a generic manner to understand the possible effects of site variability and of different boundary conditions, and not to directly generate flow fields for PA.

A scoping approach would allow more direct tracing of assumptions and the possible errors these imply, and would give the possibility of developing more confidence in the

analysis. The only way that SKI could possibly check model results of SKB, if they were directly used in the SR 97 manner in an actual license application for an SFL2 site, would be to independently and completely model the site. There may be little value added by such difficult independent modeling efforts and SKI evaluation of scoping analyses may be more effectual and thus preferable.

Glacial scenario

Climate change may have significant impact on both the flow field and the geochemistry surrounding the repository. However, the climate change scenario was not thoroughly evaluated within SR 97.

- No careful analysis was made of glacial conditions at Beberg and Ceberg, and only a local scale model evaluation was done of Aberg.
- The effects of a nearby ice front are not necessarily the only ones that need to be considered in a glacial scenario. Deep brines discharge at the coast and would follow the coast in and out. Possible brine intrusion may thus occur as the shoreline moves and during future evolution of sites, there may not only be seawater at near-coastal sites (such as Aberg), but possibly also shield brine. This would have some impact on geochemical controls (e.g. canister corrosion rates, radionuclide solubility and sorption).
- Oxygen transport to and below repository depths can easily occur given the general hydrogeologic conditions modeled as clearly shown by SKB in ground-water modeling for SR 97. This would be a key problem for the near field, increasing canister corrosion, and increasing radionuclide solubility and mobility.
    - SKB's main requirement, that geochemical conditions be reducing at repository depth, was not seriously challenged prior to Glynn and Voss (in SKI 97:13), Glynn and others (Borgholm workshop proceedings, NEA, 1999), Glynn and Voss (SKI 96:29), and SKI Site94 (SKI 96:36). They demonstrated the possibility that oxygenated glacial meltwaters could exist at repository depths for periods as long as 10 to 25 Ka during the warm-based phase for each glaciation of SKB's scenario. This may be enough time for oxygen transport though the buffer and to the canister.
    - Fluid travel times from the surface to repository depth below a glacier are only 10s to 100s of years, as demonstrated by SR 97 modeling and the work listed above.
    - Despite minor evaluation of this possibility within SR 97, consideration of possible oxidizing conditions at the repository was not considered sufficiently by SKB. One supporting report (Guimera and others SKB TR 99-19) mentions some situations in which oxygen can indeed reach repository depths.
    - SKB needs to objectively evaluate sub-glacial oxygen transport and demonstrate the robustness of the repository under these possible adverse conditions.

- There are linkages of various events that may likely occur due to glaciation that were not considered, and which may strongly impact repository function (see below).

Biosphere

The discharge points from the ground-water models that are the primary input to biosphere selection are among the least certain results of the hydrogeologic analysis. This makes it much less useful and less meaningful to apply a sophisticated biosphere approach, as it depends on highly uncertain discharge locations. A simpler more-generic biosphere approach may be more appropriate to use and more in concert with the level of certainty in the other portions of the PA.

General conclusions

If it is certain that the near-field engineered barriers are nearly perfect as assumed in SR 97, it seems that SKB's contention that site and the hydrogeologic barrier to release does not really matter would be true. Doses are orders of magnitude below the lowest level of concern, almost irrespective of other conditions, if the near field is nearly perfect.

If there is any doubt that the near field is so perfect (i.e. no more than 5 damaged canisters), then much can be questioned about many aspects of the analysis presented, possibly leading to more significant dose consequences than demonstrated in SR 97.

One source of near-field doubt stems from the consequences of combinations of scenarios in which several negative events are linked. Such a circumstance has not been considered, and for the most part, the effect of each scenario is evaluated only independently in SR 97. Disastrous breakdown of complex systems may occur due to a chain of linked failures. For the repository, an obvious linking of negative circumstances would be for the glacial scenario, for example, which gives a possibility of correlated events. These include: high ground-water flow (possible ablation of buffer and high fluid transport), change in ground-water chemistry (even the possibility of oxidizing conditions), new flow paths, significant changes in mechanical stress and possible motion along faults (which may also generate new flow paths), and so on. Each of these events may cause one or more failures and it is not unlikely that a number of these would occur together. Other failure chains could be defined for a repository under other circumstances. SR 97's treatment of correlated circumstances seems overly optimistic or simplistic, adding to doubt about the perfection of the near field.

Specifically with regard to hydrogeology, it is difficult to evaluate any contribution the hydrogeologic barrier may lend to increased safety margins on the basis of the SR 97 approach. This barrier is never allowed to be the main control on release in SR 97,

thus it is not thoroughly tested. Finally, this reviewer would reiterate that if only a few hydrogeologic parameters will finally be used for the PA, then the most appropriate values of these should be generated as directly and simply as possible. It is understandable that SKB has tried to use what is perceived as a state-of-the-art approach in quantitative hydrogeologic analyses. However, use of complex numerical modeling of ground-water flow to generate PA parameter values obscures many uncertainties and hides the combined effects of the many underlying assumptions. Such modeling is most meaningful and valuable for hypothesis testing concerning a site, and for increasing scientific intuition about complex processes. Despite it's standing as the most "advanced" technology available, complex numerical modeling, as demonstrated for SR 97, is not reliable for generating meaningful values for PA parameters in the bedrock of Sweden. Simple hydrogeologic scoping analyses may give the required PA parameter values most effectively and the underlying assumptions are obvious.

References

Dverstorp, B., Voss, C.I., and Geier, J. 1996, Simple evaluation of ground-water flow and radionuclide transport at Äspö, Swedish Nuclear Power Inspectorate Report 96:14, Swedish Nuclear Power Inspectorate, Stockholm.

Glynn, P.D., and Voss, C.I., Glaciation and ground-water geochemistry in the Fennoscandian Shield: Deep oxygenated ground water of glacial origin (abstract in: Glaciation and Hydrogeology, Workshop on the Impact of Climate Change and Glaciations on Rock Stresses, Groundwater Flow and Hydrochemistry – Past, Present, Future, Hässelby Castle, Stockholm, April 17-19, 1996. Swedish Nuclear Power Inspectorate Report 97:13, Swedish Nuclear Power Inspectorate, Stockholm).

Glynn, P.D., and Voss, C.I., 1999, Geochemical Characterization of Simpevarp Ground Waters near the Äspö Hard Rock Laboratory, Swedish Nuclear Power Inspectorate (SKI), SKI report 96:29, 210 p.

Glynn, P.D., Voss, C.I., and Provost, A.M., 1999, Deep penetration of oxygenated meltwaters from warm based ice sheets into the Fennoscandian Shield, in: Use of Hydrological Information in testing groundwater flow models: Technical Summary and Proceedings of a Workshop organized by the NEA Coordinating Group on Site Evaluation and Design of Experiments for Radioactive Waste Disposal (SEDE) and by the Swedish Nuclear Fuel and Waste Management Company (SKB), Borgholm, Sweden, September 1-3, 1997, p. 201 - 241.

SKI (Swedish Nuclear Power Inspectorate) with Voss, C.I., 1996, SKI SITE-94 – Deep repository performance assessment project: Volume I and Volume II, Swedish Nuclear Power Inspectorate Report 96:11, Swedish Nuclear Power Inspectorate, Stockholm, 660p.

A Review of Expert Judgement and Treatment of Probability in SR 97

Roger D. Wilmot
Mark B. Crawford

Galson Sciences Ltd
5 Grosvenor House, Melton Road
Oakham, Rutland, LE15 6AX, UK

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Summary

The Swedish Nuclear Fuel and Waste Management Company (SKB) recently published its latest performance assessment for deep disposal of spent nuclear fuel, based on the KBS-3 concept. This assessment, SR 97, uses three hypothetical repository sites (known as Aberg, Beberg and Ceberg) to provide a range of geological settings and hydrogeological conditions for the assessment. The long-term performance of these sites is compared for several sets of assumptions relating to canister lifetimes, climate evolution, and patterns of human behaviour.

This report is a review of SR 97 conducted by Galson Sciences Ltd on behalf of the Swedish Nuclear Power Inspectorate (SKI). The review focussed on the use of expert judgement in the assessment and on the treatment of uncertainty and the use of probability in assessment calculations.

Expert judgement plays an important role in all assessments, and is required both for making decisions about the conduct of the assessment (e.g., selection of conceptual models, treatment of FEPs) and for parameterising models where site characterisation data are absent. Because expert judgements play a key role in all aspects of an assessment, it is important that they are acknowledged, documented and appropriately justified.

The review of SR 97 concluded that SKB had identified many of the judgements made in developing and implementing the assessment and modelling approaches, but that a more formal documentation of the assumptions involved would add to the clarity and transparency of the use of judgements. Similarly, explicit acknowledgement of the basis for making judgements about the treatment of FEPs would improve confidence in the assessment. There are a number of tools that can be useful in justifying the judgements made in an assessment. The review concluded that more use of dialogue with stakeholders, peer review and expert elicitation could all be of value in SKB's assessment programme.

Recently introduced regulations in Sweden have established an individual risk criterion for the long-term performance of repositories. SKB has previously identified "pessimistic" and "reasonable" values for a number of model parameters, and used these in a range of deterministic calculations to calculate dose and to illustrate system performance. To allow for the calculation of risk, SKB introduced probabilistic analyses into the SR 97 assessment by assigning probabilities of 10% and 90% to the pessimistic and reasonable values respectively. The review considered this approach to be arbitrary and also concluded that the use of continuous probability distribution functions, rather than discrete "pseudo-distributions", would help in understanding system behaviour and building confidence.

1 Introduction

This report has been prepared by Galson Sciences Ltd. (GSL) on behalf of the Swedish Nuclear Power Inspectorate (SKI) as part of SKI's overall review of the recently published SR 97 performance assessment (PA) from the Swedish Nuclear Fuel and Waste Management Company (SKB). SR 97 provides a comprehensive description of a deep disposal system for spent nuclear fuel, based on the KBS-3 disposal concept, at three hypothetical repository sites (known as Aberg, Beberg, and Ceberg). SR 97 compares the long-term performance of these sites under different sets of assumptions regarding the longevity of the canisters, evolution of the climate, and different patterns of human behaviour.

SR 97 uses probabilistic techniques because the PA must calculate risk for comparison with the recently introduced Swedish regulatory criteria [SSI FS 1998:1]. The risk criterion states that the annual risk of harmful effects after closure should not exceed 10^{-6} for a representative individual in the group exposed to the greatest risk. Probabilistic techniques can also be of value in exploring the uncertainties inherent in the description and analysis of the disposal system. Our review covers SKB's treatment of expert judgement and SKB's approach to probabilistic calculations.

SR 97 is presented in two main volumes and in a number of supporting reports that provide information about how SKB has structured its assessment and determined the information to be included in the assessment. The following short-hand is used to refer to these reports:

- MRV – SR 97 Main Report Volumes I and II, SKB Technical Report TR-99-06 (SKB, 1999a).
- D&DU – SR 97 Data and Data Uncertainties, SKB Technical Report TR-99-09 (Andersson, 1999).
- PRE – SR 97 Processes in the Repository Evolution, SKB Technical Report TR-99-07 (SKB, 1999b).

Review objectives

SKI recently commissioned GSL to undertake a scoping study on the use of expert judgement in performance assessment for radioactive waste disposal (Wilmot and Galson, 2000). This study presented recommendations for the application and assessment of expert judgement for different elements of the PA development cycle. The current report uses the framework established by Wilmot and Galson (2000) to structure the review of the way in which expert judgements have been used in SR 97.

The review of expert judgements has three principal objectives:

- To determine how well SKB has acknowledged its expert judgements during the different elements of the PA development cycle, and how well the judgements are documented.
- To evaluate the appropriateness of the use of expert judgement by SKB during each of the different elements of the PA development cycle, and the tools used by SKB to justify the judgements.

- To make recommendations for future practice by SKB that will help SKI in reviewing the use of expert judgement in proposals by SKB for the siting, construction and operation of radioactive waste repositories.

Not every case of expert judgement in SR 97 has been reviewed in detail. Rather, key examples of types of expert judgements and the associated justification tools used at each stage of the SR 97 PA development cycle have been identified and discussed.

The review of the treatment of probability has two principal objectives:

- To evaluate how SKB has incorporated probability into its PA calculations in order to calculate risk for comparison with the SSI regulatory criterion.

- To compare the approach of SKB with international practices in probabilistic safety assessment for radioactive waste repositories, and to make recommendations for future practice.

Report structure

Section 2 of this report considers the use of expert judgement in the selection, justification, documentation and review by SKB of the assumptions that underpin SR 97. Section 3 considers the way in which SKB has incorporated probabilistic elements into SR 97. Conclusions and recommendations arising from the review are presented in Section 4.

2 Use of Expert Judgement in SR 97

2.1 Introduction

Wilmot and Galson (2000) classified expert judgements according to *why* the judgements are made and according to *how* the judgements are made. The two principal reasons why judgements are made are because alternatives are not feasible, and because there are no alternative approaches for making the decision. Feasible alternatives may not be available for measuring certain types of data because observations on the required spatial or temporal scales would be impracticable. Alternatively, the experiments required might be too expensive to conduct at a particular stage of a development programme. In contrast, the second type of judgements are required because there are no observations that could be made in place of the judgement. For example, speculation about future human activities cannot be supported by observations, and nor can judgements concerning the selection of a particular modelling approach or the scope of PA calculations.

A number of tools and methodologies are available for assessing judgements, with the most appropriate tools depending on both the type of judgement made and the stage within the PA process at which the judgement is made. This review uses the following stages of the PA process as the basis for describing the use of judgements in SR 97:

- Assessment context.
- Site selection / characterisation.
- Repository design / optimisation.
- Scenario development.
- Model development.
- Parameterisation.

The key techniques available for presenting and assessing expert judgements are documentation, quality assurance (QA), peer review, expert elicitation, and dialogue with stakeholders (Wilmot and Galson, 2000). The following sections discuss how these techniques have been used by SKB in the stages of the assessment process listed above.

2.2 Assessment Context

The assessment context is the assemblage of factors that influence the conduct of an assessment. By definition, all of the decisions made in defining the assessment context are judgements because they relate to issues that cannot be quantified by any observations or analyses, although ranking methods can be used as a means of comparing values held by different stakeholders. Stakeholders should have a role in defining the assessment context because much of the public debate will focus on overall issues and approaches rather than on the details of the technical analysis.

There is no unambiguous statement of the assessment context in SR 97, or of the judgements involved in developing it, although Sections 1, 2 and 3 of MRV describe the background to the assessment. The assessment context is strongly influenced by the applicable regulations, and the guidance published by the Swedish Radiation Protection Institute (SSI, 1999) sets out some of the assumptions and judgements involved in setting the regulations.

The assessment context, and particularly the approach of developing an assessment of three hypothetical sites, is influenced by the mission of SKB. It is not clear from SR 97 whether any dialogue was undertaken in developing this approach to fulfilling this mission, other than the formal reviews of SKB's programme by the regulators.

2.3 Site Selection / Characterisation

No final site selection is made in SR 97. However, three sites are evaluated to illustrate a range of environments that are typical for Sweden, and judgement has been exercised to determine that these three sites constitute an appropriate range. The three sites analysed are hypothetical sites, but the data used are derived from available data for three real sites. Judgements have been made in determining where sufficient site-specific data are available and where generic data should be used. These judgements will be different in an assessment of any proposed site because the option of additional site characterisation will also be available. SKB will need to provide careful documentation to demonstrate that it has transferred data from its hypothetical assessments to assessments of a potential site in a reasonable manner.

As must be the case, considerable expert judgements are involved in the acquisition and interpretation of site characterisation data at the three sites. For example, the site geological structure models presented in Section 6.1 of D&DU represent the application of expert judgement, particularly through extrapolation of direct measurements (e.g., outcrop mapping) and interpretation of indirect measurements (e.g., geophysics). The quality of the data and the approaches to interpretation vary between the sites and, therefore, so does the reliance on expert judgement. The documentation and QA of the site characterisation data and interpretation is presented in reports supporting SR 97 (e.g., Rhén *et al*., 1997) and are generally good. This allows evaluation of the models outside the project by independent peer review and by the regulator. For the purposes of SR 97, the uncertainty associated with the site structure models and, therefore, the appropriateness of the mix of data and judgement, has been evaluated by Saksa and Nummela (1998). However, more extensive peer review might be required for a real post-closure safety case.

The development of hydrogeological models for the sites is also based to a significant degree on expert judgement, particularly in the extrapolation of data from boreholes. For example, hydrological parameterisation of conductor domains at the regional scale is based on extrapolation and expert judgement (p. 60 of D&DU). The scaling of hydraulic conductivities (i.e., applying measurements to blocks of sizes larger than the measuring scale) is based on a regression analysis that "builds on a series of non-proven assumptions" (p. 61 of D&DU) or, in other words, expert judgement. However, as with the geological characterisation data, the documentation and QA of the hydrogeological characterisation and interpretation is generally good. This enables independent review of the judgements and uncertainties involved.

2.4 Repository Design and Optimisation

SR 97 is an assessment of hypothetical sites undertaken to help in understanding the effects of differences in hydrogeological regimes. To allow these differences to be analysed, it is important that certain assumptions are held constant for the three sites under study. The repository design is one such factor. In an assessment of a potential repository site, optimisation of the repository design would take account of site-specific features and would therefore be different for any site considered. For comparing hypothetical sites, it is therefore appropriate not to optimise the design. SKB has previously documented an approach to optimisation, and the judgements made in this approach, and in developing the design concept used in SR 97, are described outside SR 97 (e.g., KBS-3 (SKBF, 1983); PASS (SKB, 1992); PLAN 98 (SKB, 1998)).

2.5 Scenario Development

Wilmot and Galson (2000) sub-divided the topic of scenario development into three sub-topics:

- Derivation of a comprehensive list of features, events and processes (FEPs) potentially relevant to system performance.
- Reduction of the full FEP list to a set of FEPs to be accounted for in system calculations. This reduction should follow a screening protocol using defined screening criteria.
- Development of a set of scenarios for calculating dose, risk and other performance end-points.

Judgements are required at each stage, and the judgements made in SR 97 are discussed in the following three sections. The use of scenarios in SR 97 is discussed in Section 3.2.3 of this review. Many of the judgements regarding scenarios involve the way in which they are used in risk analyses and how they are treated probabilistically, and the comments in Section 3.2.3 should be read in association with the discussion below.

2.5.1 FEP list

SKB has previously compiled a FEP database (Andersson *et al*., 1989) and has used interaction matrices to identify processes and interactions of importance for the evolution of the repository (e.g., Skagius *et al*., 1995). In SR 97, a new structure for description of the repository system has been adopted, termed THMC (thermal-hydraulic-mechanical-chemical) diagrams. The role of these different tools in future assessments is to be evaluated and rationalised by SKB (Section 4.2.4 of MRV).

Derivation of the FEP list, interaction matrices and THMC diagrams are all based on expert judgement. This is acknowledged in Section 5.8 of MRV. Expert judgement is used because there is no ready and acceptable alternative. The judgements are made predominantly in a formal and controlled environment by working groups of technical project personnel and experienced consultants. Assessment of the expert judgement is by peer review and informal expert elicitation, and also by cross-checking between the different tools and by comparison with work of other organisations (e.g., the NEA International FEP List). However, as is

acknowledged in Section 7.3.3 of MRV, this cross-checking has not yet been undertaken in a systematic and formal manner.

Documentation of the THMC diagrams is provided in PER and in Pers *et al*. (1999). Pers *et al*. (1999) was not reviewed, but the documentation in PER is generally good. Documentation of the FEP database and interaction matrices is also good, although this work was undertaken outside the auspices of SR 97. However, documentation of the expert judgement applied in identifying the processes is not always adequate, in that only the end result has been presented and the thought processes have not always been recorded. Minutes of working group meetings may address this deficiency in part, but the minutes do not capture work done by individuals outside of the meetings.

2.5.2 FEP screening criteria and FEP screening

No formal FEP screening criteria are presented. PER presents the reasoning behind which processes are represented in the modelling of the various scenarios in SR 97; the main FEP screening criteria that have been applied are likelihood of FEP occurrence and consequences of FEP occurrence in terms of system performance. Neither of these criteria are applied in a quantified and formal manner; for example, the consequence criterion is often based on the effect on a subsystem component compared to the effect, or uncertainty associated with the effect, of another process.

Many screening decisions are the result of expert judgement relating to the review of scientific evidence and considering its relevance to the SR 97 assessment, i.e., expert judgement is used to choose between the alternatives of modelling or not modelling a process. The review process to justify the screening is generally well documented in PER. In most cases, the judgement is clear but, in several cases, there is considerable uncertainty about whether the judgement is appropriate or valid. These areas are candidates for further work to assess the judgement (e.g., erosion of the bentonite buffer, formation of colloids in scenarios where the bentonite is breached, colloid transport).

Screening judgements are often made by technically-qualified individuals. In some cases, more contentious judgements may be made by a group. In both cases, assessment of the judgement would be expected to be done predominantly by peer review. However, in SR 97, there is no identification of the responsible parties for each screening decision, other than by the naming of the managers for each section (i.e., near-field, geosphere, etc.). Further, there is no mention of any peer review undertaken outside the project.

2.5.3 Scenario development

Five scenarios are evaluated in SR 97. Section 7.3 of MRV acknowledges that scenario development is based on expert judgement and cannot be proven to be comprehensive. The scenarios chosen are justified (i.e., the expert judgement is assessed) by comparison with the scenarios selected in other assessments. In the case of unlikely events, scenario selection has also been based on an assessment of probability and whether uncertainties can be accounted for by the use of variants of a given scenario or whether an explicit scenario is required. There is no documentation of the thought processes behind scenario development and no formal verification of the comprehensiveness of the scenarios selected. Section 7.3.4 of MRV states SKB's intention to revise the set of scenarios used and to undertake a formal review of the selection process.

Wilmot and Galson (2000) emphasised dialogue with stakeholders as an important tool for assessing the selection of scenarios and screening criteria. However, the use of dialogue with stakeholders is not discussed in SR 97.

2.6 Model Development

Numerous modelling assumptions are made as part of conceptual model development and in the implementation of the conceptual models through mathematical representation, numerical solution, and code configuration. As with FEP screening, these assumptions all rely to a greater or lesser extent on expert judgement. Some assumptions are well supported by experimental evidence or modelling calculations, while others rely more on expert interpretation of how best to account for uncertainty and variability. In SR 97, description of the modelling assumptions are found throughout the documentation. PER is the main source of information. However, there is no systematic documentation of assumptions and, as with the FEP screening, there is no formal identification of the responsible person for each assumption. Because there is no systematic documentation, there can be no formal peer review of each assumption.

Some of the more significant judgements with regard to model development are made in the conceptualisation of the climate change and earthquake scenarios. This is primarily because, for these scenarios, it is necessary to bound future natural events and their consequences, and this involves considerable uncertainty. These judgements are well documented throughout SR 97.

The earthquake scenario is based on a primary judgement that large earthquakes (magnitude 7.5 to 8.5) can occur in the future and can be predicted by extrapolation of data from the limited time interval covered by instrumental recording of earthquakes. However, in this time interval, there have been no earthquakes recorded having a magnitude greater than 5.

The conceptualisation of the climate change scenario involves judgement both about the timing of events and the consequences or effects of these events. For example, with regard to timing, land uplift appears to be well characterised (Section 8.3.2 of MRV), but sea-level change predictions do not apparently account for greenhouse gas effects. The effects of glacial meltwater are based on observations of past behaviour that become less clear with time. Therefore, the model is predominantly based on behaviour since the most recent glacial event only. The model is supported by studies that seek to explain the observed groundwater distributions (e.g., Svensson, 1999) and seek to predict the magnitude of future effects (e.g., Guimera *et al*., 1999). However, judgements must be applied both to future boundary conditions, driving forces, and durations, and to assumptions that future behaviour will parallel past behaviour.

Thus, judgements on the conceptualisation of the earthquake and climate change scenarios are largely made because there is no ready alternative. Peer review and dialogue would be good methods of building confidence in the judgements, but use of these tools is not discussed in SR 97.

In SR 97, a stochastic continuum model was applied for detailed-scale hydrogeolgical modelling. There are alternative conceptual models, as set out in Section 6.3.2 of D&DU, and quantitative evaluation of these alternatives has been performed to support the choice of the main modelling technique (Section 6.5.4 of D&DU). However, the choice of modelling

technique also relies partly on expert judgement which, in turn, is influenced by available tools and data. The application of the stochastic continuum model itself requires expert judgement, and this has been undertaken in part by a working group (Section 6.5.3 of D&DU). The basis for the modelling decisions taken is well documented in supporting reports (e.g., Walker and Gylling, 1998; 1999; Selroos and Ström, 1999).

2.7 Parameterisation

The derivation of parameter values for the SR 97 calculations and the associated uncertainty is documented mainly in D&DU. Section 2.1.3 of D&DU discusses the treatment of probability and acknowledges that subjective uncertainty can be treated using probability distributions for parameter values, and that such distributions are often constrained by expert judgement. However, the approach taken in SR 97 is to use, where possible, "reasonable" and "pessimistic" estimates of parameter values, rather than probability distributions. Section 2.2 of D&DU acknowledges that the derivation of both reasonable and pessimistic values is judgmental. Section 2.2.3 of D&DU states that probability distributions are only presented where there are data to support the distribution.

The expert judgements made or presented in D&DU mostly concern derivation of parameter values that describe physical attributes of the disposal system from a range of site characterisation, experimental and literature data. D&DU appears to be the primary documentation to support this process and is the main link between the judgements and the supporting data references. The process of deriving parameter values for assessment calculations does not appear to have been formalised under appropriate QA procedures so as to ensure a consistent and adequate documentation. Further, there is no evidence of formalised independent peer review to build confidence in the judgements, although several SKB reports reflect peer review undertaken within the project to review data and uncertainties in SR 97 (e.g., Bruno and Duro, 1997; Follin, 1999). The judgements are sometimes made by the author of D&DU (e.g., the instant release fraction) and sometimes by individuals or groups of technical experts in supporting reports (e.g., solubilities reported in Bruno *et al*., 1997). Despite the usefulness of formal elicitation for dealing with uncertainty, none has been performed.

Informal group elicitation is only mentioned in Section 4.3.2 of D&DU, where the use of expert judgement, or "speculation," to determine the size and frequency of initial canister defects is discussed. The expert judgement is stated to be based, in part, on elicitation of SKB staff. However, there is no documentation of this elicitation process, e.g., who took part, who conducted the elicitation, how it was conducted, what questions were asked, and what answers were given. Therefore, the suggested reasonable and pessimistic parameter values are not traceable to source. Furthermore, in the Appendix of D&DU, Table A.1.3.1 gives a probability distribution for the number of canisters with initial defects, despite the statement that probability distributions would only be provided where there are data or other well founded means to support the distribution.

Section 5.6 of D&DU discusses the derivation of sorption data for the geosphere. The use of expert judgement to select which experimental data to use is acknowledged. This judgement is presumably documented in the supporting SKB report that describes the derivation of the sorption database (Carbol and Engkvist, 1997 – this report was not available to this review). The judgement used by Carbol and Engkvist (1997) is questioned, both by the author of D&DU and by a SKB-funded peer review of the data (Bruno and Duro, 1997). The dismissal

of the influence of temperature, organics and variable mineralogy and the use of chemical analogy appear to be based on judgement rather than data. However, no major changes to the parameter values provided by Carbol and Engkvist (1997) were recommended, and the values were unchanged for use in SR 97. Although probability distributions were not used in SR 97, Carbol and Engkvist (1997) did provide uncertainty ranges in their sorption data, and D&DU recommends that a uniform distribution should be applied to these ranges for probabilistic calculations. No basis for this recommendation is provided, and it appears to be based solely on the judgement of the author of D&DU. However, a log-uniform distribution rather than a uniform distribution has been shown to be more appropriate for sorption data in soils (e.g., Sheppard and Thibault, 1990) and in limestone (EPA, 1998). Therefore, the possibility of a log-uniform distribution should at least have been evaluated and documented in making the judgement of which distribution type to apply.

3 Use of Probabilities in SR 97

3.1 Introduction

SSI has recently introduced a risk criterion into the regulations that apply to the disposal of spent fuel. The regulation and the accompanying guidance indicate that the regulatory authorities require a consideration of both consequences (doses) and the probability of receiving a dose to be considered in assessments. This review is concerned primarily with the way in which SKB has determined probabilities and incorporated these into SR 97. The review has, to some extent, been broadened to consider SKB's overall approach to risk assessment. This widens the scope because a risk assessment is not just a means of demonstrating compliance with a risk criterion, but is also a means of developing and documenting an understanding of system behaviour and of the associated uncertainties.

In the context of demonstrating compliance, the disposal concept developed by SKB is sufficiently robust that performance assessments show that only low doses would arise in the majority of foreseeable futures, and that the probability of circumstances that could lead to doses above the prescribed limits are sufficiently low that the overall risks are well below the regulatory target. This report presents some comments on the way in which SKB has used probabilities in their analyses and presentation of results. We do not anticipate that addressing these comments would result in an average calculated risk greater than the regulatory limit, although some risks may increase if parameter distributions are treated differently. However, we believe that a clearer explanation in a number of places would improve the transparency of the analyses and increase confidence in the overall assessment.

SR 97 is the latest in a series of performance assessments undertaken by SKB to develop understanding of system behaviour for three hypothetical disposal sites. Previous assessments have concentrated on comparing performance with the dose criteria previously included in Swedish regulations, and have also used deterministic calculations involving pessimistic assumptions.

In SR 97, SKB has recognised the need to consider probabilities in determining risk, but has not developed a coherent risk methodology. Instead, SKB has simply assigned some arbitrary probabilities to their existing assumptions, and attempted to justify this by noting that a fully probabilistic approach is difficult to implement. It would not be reasonable, given the recent introduction of a risk criterion, to expect SR 97 to demonstrate a fully-developed probabilistic risk assessment methodology. However, we believe that it would have been reasonable for SKB to have noted the lack of time to develop a probabilistic approach, to have outlined a methodology for future assessments, and to have presented a work programme for implementation.

3.2 Accounting for Uncertainty

Before discussing the ways in which uncertainties are treated in performance assessments and, in particular, the way in which probabilistic approaches are used, it is useful to discuss the different types of uncertainty that need to be addressed. Three principal sources of uncertainty are commonly identified:

- **Parameter uncertainty**: This type of uncertainty arises because knowledge about a site, including the characteristics of the geological setting and the conditions within the repository, can never be fully known. Even where measurements and observations are made at the site, they cannot account for all of the spatial and temporal variability within a natural system or a complex chemical environment. In many cases the data used are not site-specific and uncertainties arise in applying generic data to a particular site.

- **Conceptual model uncertainty**. This type of uncertainty arises because there can be alternative models that explain the behaviour of parts of the disposal system and the interactions between the features, events and processes that operate within the disposal system.

- **Scenario uncertainty**. This type of uncertainty arises because the evolution of the environment around a disposal system is unknown. This environment defines the initial and boundary conditions of the disposal system, and assumptions about its evolution are required before analyses of disposal system behaviour can be conducted. Different sets of assumptions (scenarios) provide broad-brush descriptions of the future environment.

The distinction between these types of uncertainty is not absolute, and judgements are required to classify uncertainties. Nevertheless, these types of uncertainty are often treated differently in PAs, including SR 97, and the majority of this review uses this classification.

Risk is a useful criterion for assessing the performance of any system in which the outcome is uncertain, because the language of risk can also be used to characterise uncertainty. As an example, at low radiation doses, the consequences to individuals in terms of the onset of cancers are uncertain: there is a small probability that an exposed individual will develop cancer. If the level of the exposure is known, then this probability is the only contributor to the risk. If the level of exposure is uncertain, then additional probabilities that express the other uncertainties can be used to determine risk.

SKB is correct in noting that, for a system such as a deep disposal facility for spent fuel, frequency data are not available to characterise most uncertainties. Other techniques, many involving use of expert judgement, are required to express conceptual model and scenario uncertainties as probabilities, and also a large proportion of the parameter uncertainties. SKI and SSI recently held a seminar to consider the ways in which these expert judgements could be captured and used (Wilmot *et al*., 2000).

3.2.1 Parameter uncertainty

Instead of using available information and expert judgement to characterise parameter uncertainty using probability distributions, SKB has adopted the concept of "reasonable" and "pessimistic" values to define uncertainty. These two values have been determined using a variety of group and individual judgements, with varying degrees of documentation and traceability (see Section 2). The use of the concept of reasonable and pessimistic values is not, in itself, inappropriate. SKB has, however, applied arbitrary and unjustified probabilities of 90% and 10% to the reasonable and pessimistic values respectively. SKB's approach to probability assignment does not accord with that used in any other PA programme, and we do not consider it appropriate either for presentation of a safety case or for regulatory decision-making.

As well as assigning arbitrary probabilities for the two values it has selected, SKB has also used the resulting "pseudo-distribution functions" inappropriately. In SKB's methodology, if there were only two uncertain parameters, A and B, there would only be four parameter combinations to consider - A(p):B(p); A(r):B(r); A(p):B(r); and A(r):B(p), where r represents the reasonable value and p the pessimistic value of the parameter. In a calculation involving 100 realizations, these combinations would occur, on average, 1, 81, 9 and 9 times respectively. No additional information or understanding would be gained, however, by repeating one calculation 81 times, and the output from such a calculation would be limited to four discrete values.

A better approach to probabilistic analysis than that adopted in SR 97 would be to use the two estimated values to define points on a continuous distribution function for each parameter. Sampling from this function would then include values other than the two fixed values in the analysis.

If sampling from a continuous distribution function is undertaken, there are better, and less arbitrary, functions than those defined by SKB's reasonable and pessimistic values. Two such distributions are the uniform and triangular distributions, neither of which require onerous levels of expert judgement or elicitation to define, but which can be used to build an understanding of system behaviour and determine sensitivities.

In the uniform distribution, a minimum and a maximum value are defined, and all values between these are assumed to be equally probable. SKB's "pessimistic" values could be regarded as the maximum value, but a minimum (optimistic) value must also be determined. Minimum and maximum values are also required for a triangular distribution, together with a median value. SKB's "reasonable" values could be treated as the median value, although some re-assessment might be required where the reasonable value accords more closely with the modal value of the distribution.

Figure 9-41 of MVR shows that the form of the distribution function is not critical for a number of parameters, since there is little relative change in the calculated dose when the parameter value is varied between "reasonable" and "pessimistic". However, for a number of parameters there is a significant change in calculated dose. In a system in which there are non-linearities, simple interpolation cannot be used to infer the behaviour of the system for values between these limits. Defining uncertainties using a probability distribution function (pdf) would allow for proper sampling across the range of values. For example, if triangular distributions were used for two parameters, each realization would involve different parameter values, with values close to the maximum, between median and maximum, just above the minimum, etc., being sampled, as well as just the end-point values. It is likely that the "steps" apparent on the cumulative doses curves (e.g., Fig. 9-44 of MVR) would be resolved by this approach.

It is unlikely that sampling from continuous probability density functions instead of discrete ones would lead to a major change in calculated doses and risks. However, the purpose of a performance assessment is not solely to demonstrate compliance with regulations but is also to develop an understanding of system behaviour and identify areas where further research and development should be focussed. As well as being less arbitrary, the use of continuous functions rather than the two-valued, pseudo-distribution functions, at least for the sensitive parameters, will allow for a much clearer understanding of system behaviour.

3.2.2 Conceptual model uncertainty

SKB acknowledges that there is uncertainty associated with the selection of conceptual models for use in PA calculations. There are useful discussions of the different conceptual models for several parts of the disposal system in D&DU. These provide the basis for SKB's selection of a single conceptual model and, in general, the selection is based on the model that is assessed to be reasonable. The alternative approach - assigning probabilities to the different conceptual models and using these to control how the models are used in PA calculations - is not used. The selection of a single conceptual model is not inappropriate, although it may be difficult to justify that a particular model is "reasonable". Assigning probabilities or degrees of belief to models does require expert judgement and may not be justified except in situations where regulatory decisions or optimisation depend on the choice of conceptual model.

The remainder of this section discusses two examples of conceptual model uncertainty in SR 97 that illustrate SKB's approach.

In D&DU Section 4.1, SKB describes the assumptions used to determine the inventory for each fuel element. Alternative sets of assumptions for the rate of burn-up are identified, as are alternative computational models for determining the actinide composition of spent fuel given these different assumptions. These uncertainties are not quantified, although the text implies that the alternative conceptual models can lead to uncertainties of up to 20%. SKB assumes, on the basis of preliminary and unreferenced PA calculations, that these uncertainties can be neglected because the overall disposal system is not sensitive to the original inventory. SKB also states that there is no motivation for use of a pessimistic case.

A probabilistic approach to defining the inventory for use in PA calculations would require assigning degrees of belief to the assumptions regarding burn-up and to the appropriateness of the burn-up codes. This approach would ensure that calculated inventories were self-consistent in terms of the relationships between actinides. SKB correctly notes that assigning uncertainty ranges directly to actinide concentrations is inappropriate where there are strong correlations between the concentration of different actinides. Neglecting uncertainties in the inventory and using a fixed inventory is an appropriate approach if the overall radionuclide release calculations are not sensitive to the uncertainties in the initial inventory. Given the approach used elsewhere in SR 97, however, it is unclear why the fixed inventory was not defined using pessimistic assumptions. In this case, a pessimistic value would not overly influence the overall assessment, but would provide confidence that the final performance assessment, based on the disposed inventory, would not indicate greater releases than preliminary assessments.

In the case of modelling dissolution of the UO_2 matrix, SKB discusses two conceptual models - immediate dissolution (the so-called "instant coffee" model) and a model based on a realistic description of fuel oxidation. The immediate dissolution model is discounted as being too pessimistic. However, uncertainties are not considered in the oxidation model so that only a single value of the dissolution rate is derived for use in PA calculations. This is despite SKB's observation that there are a number of assumptions in this model that could affect the dissolution rate.

3.2.3 Scenario uncertainty

Scenario definition

SKB has identified four aspects of the disposal system (or FEPs) as being outside the domain of parameter uncertainty, and has explored the effects of these on system performance by including them in separate scenarios rather than by defining "reasonable" and "pessimistic" parameter values. These scenario-forming FEPs are:

- Canister defects.
- Climate change.
- Earthquakes.
- Human intrusion.

The majority of the work presented in SR 97 focuses on system performance for the so-called base case scenario. In this case, the climate is assumed to be constant and similar to the present-day climate, land uplift continues at the current rate but there are no earthquakes large enough to affect the disposal system, there is no human intrusion into the disposal system, and there are no initial defects in the canisters. Four additional scenarios incorporate the effects of each of the above FEPs. The results of these scenarios allow the effects of different assumptions to be assessed, and therefore help in developing an understanding of system behaviour. However, there are no analyses that show the influence of interactions between these FEPs. For example, the effects of earthquakes under climate conditions other than present-day, or the effects of initial canister defects on doses received following intrusion, are not explored.

The approach of defining different scenarios to explore the influence of different sets of assumptions is a common one in performance assessment programmes. However, accounting for scenario uncertainty in risk assessments is conceptually difficult because it requires that an exclusive and exhaustive set of scenarios can be defined. Each scenario in such a set would be independent, so that the consequences could be calculated independently of other scenarios and a probability of occurrence determined. The set of scenarios would define all possible futures within the analysis domain, so the sum of the probabilities would be one and the results could be combined into an overall measure of risk. Although exclusive scenarios are relatively easy to define, it is difficult to define an exhaustive set if different events define different scenarios, because the interactions between different aspects of the disposal system are not accounted for. If an exclusive and exhaustive set of scenarios is not defined, then the calculations can only yield a set of contingent risks. Contingent risk calculations can be useful in cases where highly uncertain events can have significant consequences. For example, events such as future human intrusion can dominate calculated risks, but require speculation to define the associated uncertainties. Including human intrusion in a separate scenario will lead to contingent risk estimates, but will ensure that there is a clear separation of speculation and other sources of uncertainty, and so provide a stronger basis for regulatory decision-making.

SSI has recognised the speculative nature of probabilities for human intrusion, and states in its guidance for the risk criterion (SSI, 1999; Section 2.6.1) that:

> Questions relating to intrusion will be handled by SSI separately from the discussion concerning the undisturbed repository. Therefore, the stipulations concerning the holistic approach and optimisation in § 4 and in Section 2.3.3 shall not apply to intrusion into a repository. Estimated probabilities concerning human intrusion in the future are so uncertain that SSI does not wish to disregard requirements on the safety of the undisturbed repository.

SSI does not, however, recognise that there are any other scenarios that should be assessed through the calculation of contingent risks. SSI's guidance assumes that both consequences and probabilities can be assigned to scenarios (SSI, 1999; Section 2.4.4):

> Instead, the risk must be assessed from the risk scenario which is obtained by weighing together consequences and probabilities for different event sequences. In this context, the concept of the risk scenario refers to calculated, or otherwise assessed, consequences and probabilities for a relevant selection of possible event sequences (scenarios). The consequences must be calculated or estimated so that they include uncertainties in the assumptions and data upon which the calculations or assessments are based. The chosen scenarios must in their entirety give a full picture of the risks attributable to the final repository.

The only way in which the probabilities of scenarios can be determined in a way in which they can be used to calculate risk is if they are distinguished by the occurrence of events that can, in turn, have probabilities assigned to them. This is the approach that was used in the trial assessments undertaken on behalf of Her Majesty's Inspectorate of Pollution (HMIP) in the UK (Sumerling *et al*., 1992). A similar approach has been used for the Waste Isolation Pilot Plant (WIPP) in New Mexico (DOE, 1996). In the HMIP approach, a simulation code (TIME4) was used to generate a set of climate sequences, each of which effectively defined a "calculational scenario". For the WIPP, "calculational scenarios" were defined by sampling for the occurrence of future drilling and mining events. In both cases, the overall scenario was assumed to have a probability of one, and each realization or calculation was assigned a probability equal to the reciprocal of the number of realizations. The probabilities used in these assessments are therefore not "real" probabilities, but rather mathematical constructs dependent on the details of the calculation. The important aspect of these approaches, which enables probabilities to be defined, is that the assessments include all of the significant events within one scenario rather than treating them as variants to a base case. This ensures that interactions between uncertain events are included in the calculations, and that, within the assessment context, an exhaustive and exclusive set of (calculational) scenarios can be defined.

The approach described in SR 97 does not fulfil SSI's guidance on treatment of scenario uncertainty. The scenarios defined by SKB are mutually exclusive, in the sense that they do not overlap, and so probabilities of occurrence could theoretically be assigned. However, these scenarios are not exhaustive, because they do not consider interactions, and so the probabilities would not add to one. This means that combining results from the different scenarios would not give rise to an overall estimate of risk. In fact, the probability of occurrence of any of the scenarios analysed is essentially zero because there is a vanishingly small probability that climate conditions will remain constant over hundreds of thousands of years. Although the results of SKB's calculations are useful in developing system understanding, they cannot be combined in any meaningful manner to provide an estimate of risk as required by the regulations.

Canister defect scenario

This scenario differs from the base case scenario primarily in whether the calculations assume that defects are present in the canisters at the time of deposition. In the base case

scenario, all of the canisters are assumed to be intact at the time of deposition, and even the most pessimistic corrosion rate assumed gives a canister lifetime of about 10 million years. This means that there are no releases of radionuclides to the geosphere over the period of regulatory interest. In contrast, in the canister defect scenario, some canisters are assumed to have initial defects and these result in releases of radionuclides that eventually lead to activity levels in the biosphere sufficiently high to give doses. SKB assumes that the highest proportion of canister defects is about 0.1% (5 canisters), and that the most probable ("reasonable") value is one defective canister in the repository.

SKB has conducted dose calculations for the canister defect scenario, and has presented the results of these as risk calculations (see Section 3.3.1). Apart from the human intrusion scenario, these are the only dose calculations reported in SR 97. SKB has apparently concluded, therefore, that the canister defect scenario fulfils the regulatory requirement for accounting for all sources of risk. This may be appropriate if climate change and earthquakes can be justifiably screened out of the assessment. However, regulatory assessment would be easier if SKB clearly presented within their documentation a description of the repository system that they believe incorporates all the significant features, events and processes, and presented dose and risk calculations based on this description. Supporting analyses, such as those currently included in the base case, climate change and earthquake scenarios, should still be included to demonstrate an understanding of the disposal system and to provide confidence in the analyses.

Human intrusion scenario

SR 97 includes an analysis of the ways in which societal evolution could lead to sufficient loss of knowledge about radioactivity and the location of a repository that unintentional human intrusion could occur. SKB's conclusions are that there are circumstances in which intrusion could occur in the future, and that the most likely form of this intrusion is deep drilling. SR 97 presents analyses of the consequences to both members of a drilling crew and future residents of the site after drilling, and also discusses the probability of the human intrusion scenario.

Although the discussion of societal evolution and doses from drilling are interesting, SSI's guidance suggests that the only regulatory requirement is for an assessment of disposal system performance after an intrusion (SSI, 1999; Section 2.6.1):

> In the case of a repository, the consequences of intrusion must be described. The essential point is not to describe the chain of events that leads to the intrusion, but to study the ability of the repository to isolate and retain the radioactive substances after an intrusion, in accordance with §§ 8 - 9 of the regulations.

SKB has used an assessment of drilling rates in Sweden to determine the risks from human intrusion, but presents this as an assessment of the probability of the scenario, rather than as the probability of a drilling event. This is an example of the overlap between different types of uncertainty. If human intrusion were to be included in an overall risk assessment, then the probability of the human intrusion scenario would be relevant. On the other hand, if contingent risks are calculated, it is only probabilities *within* the scenario that are relevant.

SKB has made erroneous assumptions in determining probabilities of drilling into a repository. SKB has determined two probabilities: the probability that a randomly drilled borehole within Sweden is within the repository footprint, and the probability of a borehole within the footprint intercepting a canister. The product of these two probabilities (5×10^{-8})

is therefore the probability that any one borehole will intercept a canister. SKB then states that if 200 boreholes are drilled in Sweden each year, then during a period of one hundred thousand years the probability of intercepting a canister at some time is 1. This is erroneous, as is clearly shown by considering a drilling rate of 300 boreholes per year – during a period of one hundred thousand years, SKB's approach would give a probability of intercepting a canister of 1.5, which is nonsensical.

If SKB does present risks from human intrusion, in addition to an assessment of consequences, then it should use a Poisson function to determine the probability of intercepting a canister. Using SKB's assumptions about drilling rates in Sweden and the size of the repository footprint, this would give a probability of interception within one hundred thousand years of 0.63. After a million years, the probability would be greater than 0.999, but no random process can ever lead to a probability of exactly 1.

3.3 Risk Analyses

Section 3.2 discusses ways in which probability can be used to express uncertainties in different aspects of an assessment. This section discusses how the these probabilities are combined with a measure of consequence to give a value for risk that can be compared to a regulatory criterion.

3.3.1 Use of dose rather than risk

The concept of risk requires an assessment of both the consequence of an event or process and the probability of that event or process occurring. The consequence used in defining the risk criterion in the Swedish regulations is the incidence of fatal and non-fatal cancers and hereditary damage. At the levels of radiological dose likely to arise from a KBS-3 type repository, two probabilities are necessary to determine the overall risk - the first is the probability that some event, or process or combination of events and processes will lead to a dose, and the second is the probability that this dose will lead to a harmful effect. The International Commission on Radiological Protection (ICRP) uses a variety of information sources to determine the relationship between radiological dose and harmful effects, and its current best estimate of the probability is 0.073 per Sv.

An alternative approach to using the ICRP dose-risk conversion factor is to express the risk criterion in terms of an annual dose equivalent. This is the approach used by SKB in their presentation of results from probabilistic calculations (Section 9.11.9 of MVR). Although these two methods of presentation are essentially equivalent, there is some potential for confusion, particularly if terms such as "risk limit" and "calculated risks" are used on plots of annual dose (e.g., Figures 9-43, 9-44 and 9-45 of MVR). Since the regulatory criterion is expressed as an annual individual risk, the results of an assessment should be presented in terms of risk. Dose equivalents can also be used, but they should be used for comparisons - for example, with doses from natural background radiation.

3.3.2 Contingent risks

A contingent or conditional risk analysis is one in which the probability of some events or processes is assumed to be one. Ideally, a risk assessment would account for all the uncertainties within the system under study. In practice, and particularly in the case of

complex systems such as radioactive waste disposal facilities, use of contingent risk analyses may allow for greater transparency by simplifying the calculations.

It is important when presenting contingent risk calculations that it is made clear what assumptions have been made and that probabilities have been set to one. Contingent risks cannot be directly summed, and they are most useful for comparisons, in the sense of showing that the risks arising from one set of events and processes are greater than those from another set. If risks are to be summed, or an assessment made of the contribution of a set of events and processes to the overall risk, then contingent risks are inappropriate and the probability of occurrence must be included in the analysis.

The risk calculations presented by SKB (Figures 9-43, 9-44 and 9-45 of MVR) appear to represent contingent risk calculations, although the figure captions and explanatory text do not clearly state which probabilities have been assumed to be one. As discussed in Section 3.2.3, although there is discussion of scenario uncertainty and the probabilities of various events, SR 97 does not include a clear description of the risks arising from all significant events and processes. We consider that this is acceptable at this stage of the analysis, because risk estimates may require revision in the light of future research. We also consider that it is appropriate to distinguish between the risks associated with the normal evolution of the disposal system and those associated with intrusion into the repository after the failure of institutional controls. We do not consider, however, that an assessment restricted to contingent risk calculations is appropriate as this neglects a significant part of the uncertainties that the regulators intend should be addressed by setting a risk criterion. We do not see evidence in SR 97 of how SKB intend to address scenario uncertainties and present a risk calculation appropriate to a safety case.

3.3.3 Calculational approach

SKB presents cumulative distribution functions of calculated risk at the three sites for two different biospheres (Figures 9-43 and 9-44 of MVR). These are based on a number of realizations, each of which calculates dose as a function of time. Each realization represents a set of parameter values that are either set at the "pessimistic" value for the parameter, or sampled from the pseudo-distribution function (see Section 3.2.1). Setting parameters to their pessimistic values should ensure that the calculated risks are larger than those that would be determined if the same parameters were sampled or set to their reasonable value. However, an important aim of a risk analysis is to aid in developing an understanding of system behaviour, and using pessimistic values will not help in this respect. We consider that SKB should endeavour to overcome the technical difficulties that SKB considers are associated with the establishment and sampling of pdfs, and that are stated to be the reason for this approach.

SKB does not report the number of realizations used in its calculations of risk. In general, increasing the number of realizations increases confidence that the analyses fully cover the possible combinations of parameter values, and the confidence limits on the mean become narrower. There are a number of "stopping rules" that can be applied to determine how many realizations are required for a particular level of confidence (e.g., Orford *et al.*, 1991). These rules are based on sampling from continuous pdfs. SKB's use of distribution functions that have only two possible values ("reasonable" and "pessimistic") severely restricts the number of possible parameter value combinations, and thus many fewer realizations will be needed for a particular level of confidence than if sampling were done across a continuous pdf. Even

if SKB persists with the approach of discrete, two-valued distributions, the number of realizations should be stated and justified.

Each realization in SKB's risk analysis yields a distribution of consequence (dose) as a function of time (examples are shown in Figures 9-28 to 9-40). SKB uses the maximum consequence from each realization, at whatever time this maximum occurs, as the measure of consequence for determining risk. This is an acceptable approach to defining risk, although it does not indicate the way in which risk varies with time. As with many of SKB's assumptions and procedures, this approach tends to maximise calculated risk in comparison with other approaches that could be used.

An alternative approach to calculating risk is to determine the mean risk at particular times. Calculations of dose are generally made using numerical models rather than analytical solutions. The output of these models is not a continuous function of dose against time, but rather a set of doses calculated for specific times (e.g., 5 000, 10 000, 250 000 years). Doses at intermediate times can be interpolated to generate dose-time curves. Each realization will generally use the same set of times or, if different time steps are used, doses at a standard set of times can be interpolated. A mean dose or risk can then be calculated from the results for each realization at each time. These results, with appropriate confidence limits, will show how mean risk changes with time.

4 Key Recommendations

This review of the use of expert judgement in SR 97 and of SKB's approach to the use of probabilities leads to the following key recommendations. We consider that adoption of these recommendations by SKB would lead to an assessment that would satisfy the recently introduced risk criterion, as well as being more traceable. Such an assessment would build confidence in the KBS-3 disposal concept.

Expert judgement

A formal documentation of modelling assumptions, including classification of assumptions (e.g., conceptual, mathematical, numerical, reasonable, conservative, simplifying), would add clarity and transparency by explicitly setting out all of the expert judgements.

Documentation of FEP screening, modelling assumptions, and parameter value derivations should identify both the individual or group responsible for the work and the associated judgements, and the individual or group that has reviewed or approved the work.

Clear FEP-screening criteria are needed (e.g., low consequence, low probability). Well-defined criteria would clarify the basis for the expert judgements made in establishing an assessment model.

Three tools that appear to have been under-utilised in SR 97 are dialogue with stakeholders, independent peer review and expert elicitation:

- Dialogue with stakeholders would be of particular benefit in determining the assessment context and in scenario development. Dialogue would build confidence in the structure of the assessment and in the scenarios selected by expert judgement.

- Peer review has been used in the development of FEP lists used in SR 97, but independent peer review could be used at several other points within the assessment process, particularly as part of the model development process.

- Formal and documented elicitation could be used for particularly contentious issues that can only be readily tackled using expert judgement (e.g., climate change, canister defects).

Treatment of probability

SKB should develop a more coherent approach to risk analysis and integrate this with its assessment methodology. A key part of this approach should be a more rigorous and less arbitrary method for incorporating parameter uncertainty into the analysis. Risk analyses should place less emphasis on the use of "pessimistic" parameter values and other conservative assumptions.

SKB should describe more clearly the set of FEPs, FEP interactions, and conceptual models that it considers incorporates all of the significant uncertainties. This set of assumptions should be the basis of the risk analysis and fulfil the regulatory requirements for an integrated assessment. SKB should continue to develop and describe supporting models that help to justify its assessment models and provide confidence in its assessments. These supporting

models and results should, however, be more clearly distinguished from the assessment calculations.

In line with regulatory guidance, SKB should continue to treat human intrusion separately from other events affecting the disposal system. SKB must, however, correct its erroneous approach to determining the probability of intrusion.

5 References

Andersson, J. 1999. SR 97. Data and data uncertainties. Compilation of data and data uncertainties for radionuclide transport calculations. SKB Technical Report TR-99-09. SKB, Stockholm.

Andersson, J., Carlsson, T., Eng, T., Kautsky, F., Söderman, E. and Wingefors, S. 1989. The joint SKI/SKB scenario development project. SKB Technical Report 89-35. SKB, Stockholm.

Bruno, J. and Duro, L. 1997. Discussion of data uncertainties, Review of selected sorption data of radionuclides in granitic rock. SKB Report U-98-06. SKB, Stockholm.

Bruno, J., Cera, E., de Pablo, J., Duro, L., Jordana, S. and Savage, D. 1997. Determination of radionuclide solubility limits to be used in SR 97. Uncertainties associated to calculated solubilities. SKB Technical Report 97-33. SKB, Stockholm.

Carbol, P. and Engkvist, I. 1997. Compilation of radionuclide sorption coefficients for performance assessment. SKB Report R-97-13. SKB, Stockholm.

DOE (U.S. Department of Energy) 1996. Title 40 CFR Part 191 Compliance Certification Application for the Waste Isolation Pilot Plant, October 1996. DOE/CAO-96-2184. DOE, Carlsbad, NM.

EPA (U.S. Environmental Protection Agency) 1998. Technical Support Document for Section 194.14: Assessment of K_ds used in the CCA. EPA Air Docket A-93-02, Item V-B-4, May 13, 1998. EPA, Washington, DC.

Follin, S. 1999. Hydrogeological boundary setting in SR 97. Uncertainties in regional boundary settings and transfer of boundary conditions to site-scale models. SKB Report R-99-45. SKB, Stockholm.

Guimera, J., Duro, L., Jordana, S. and Bruno, J. 1999. Effects of Ice Melting and Redox Front Migration in Fractured Rocks of Low Permeability. SKB Technical Report TR 99-19. SKB, Stockholm.

Orford, J.L., Hufton, D. and Johnson, K. 1991. Report on some methods of determining the state of convergence of Monte Carlo risk estimates. UK Department of the Environment Report DoE/HMIP/RR/91.015. DoE, London.

Pers, K., Skagius, K., Södergren, S., Wiborgh, M., Hedin, A., Moren, L., Sellin, P., Ström, A., Pusch, R. and Bruno, J. 1999. SR 97 - Identification and structuring of process. SKB Technical Report TR-99-20. SKB, Stockholm.

Pusch, R. and Börgesson, L. 1992. PASS - Project on Alternative Systems Study. Performance assessment of bentonite clay barrier in three repository concepts: VDH, KBS-3 and VLH. SKB Technical Report 92-40. SKB, Stockholm.

Rhén, I., Gustafson, G., Stanfors, R., Wikberg. P. 1997. ASPO HRL - Geoscientific evaluation 1997/5. Models based on site characterisation 1986-1995. SKB Technical Report 97-06. SKB, Stockholm.

Saksa, P. and Nummela, J. 1998. Geological-structural models used in SR 97. Uncertainty analysis. SKB Technical Report TR-98-12. SKB, Stockholm.

Selroos, J.O. and Ström, A. 1999. The alternative modelling project: Phase 1, Evaluation report in groundwater flow and modelling of the Aberg Site. SKB Report – in progress.

Sheppard, M.I. and Thibault, D.H. 1990. Default soil solid/liquid partition coefficients, K_ds, for four major soil types: A comparison. Health Physics, 59, 471-482.

Skagius, K., Ström, A. and Wiborgh, M. 1995. The use of interaction matrices for identification, structuring and ranking of FEPs in a repository system. Application on the far-field of a deep geological repository for spent fuel. SKB Technical Report 95-22. SKB, Stockholm.

SKB (Swedish Nuclear Fuel and Waste Management Company). 1998. PLAN 98 - Costs for management of the radioactive waste from nuclear power production. SKB Technical Report 98-07. SKB, Stockholm.

SKB (Swedish Nuclear Fuel and Waste Management Company). 1999a. SR 97 Main Report Volumes I and II. SKB Technical Report TR-99-06. SKB, Stockholm.

SKB (Swedish Nuclear Fuel and Waste Management Company). 1999b. SR 97 Processes in the Repository Evolution. SKB Technical Report TR-99-07. SKB, Stockholm.

SKBF (Swedish Nuclear Fuel Supply Co. / Division KBS). 1983. Final storage of spent nuclear fuel - KBS-3. Summary. SKBF, Stockholm.

SSI (Swedish Radiation Protection Institute). 1999. Health, Environment and Nuclear Waste: SSI Regulations and Comment. SSI Report 99:02. SSI, Stockholm.

Svensson, U. 1999. A numerical simulation of the origin and composition of the groundwater below Äspö. SKB Report R-99-39. SKB, Stockholm.

Walker, D. and Gylling, B. 1998. Site-scale groundwater flow modelling of Aberg. SKB Technical Report TR 98-23. SKB, Stockholm.

Walker, D. and Gylling, B. 1999. Site-scale groundwater flow modelling of Ceberg. SKB Technical Report TR 99-13. SKB, Stockholm.

Wilmot, R.D. and Galson, D.A. 2000. Expert judgement in performance assessment. SKI Report 00:4. SKI, Stockholm.

Wilmot, R.D., Galson, D.A. and Hora, S. 2000. Expert judgements in performance assessments: Report of an SKI/SSI Seminar. SKI Report (in press).

Appendix 1 - Reviewers

Dr. Mark Crawford

Dr. Mark B. Crawford is a Senior Consultant at Galson Sciences Ltd. He has degrees in Geology and Geochemistry from Oxford University (BA) and Leicester University (PhD), and a Diploma in Environmental Impact Assessment. Over the last nine years he has been involved in consultancy and research work in the area of radioactive waste disposal for clients in Finland, France, the UK and the US. This work has included the development of geochemical models for organic complexation in natural systems, validation of sorption modelling within a European Community research initiative, and interpretation of hydrochemical data obtained as part of Nirex's site characterisation programme. He has performed reviews of geochemical techniques in relation to palaeo-hydrogeological studies and of the effects of alkaline plume migration from cementitious waste repositories. He made substantial contributions to the development and review of technical input for the Waste Isolation Pilot Plant (WIPP) Compliance Certification Application, and subsequently in responding to stakeholder comments. He has undertaken review and systems analysis of the WIPP near-field modelling, and helped in development of compliance monitoring strategies. He was involved in a review of scenario development methodologies on behalf of ANDRA in France, and was the lead author for a report describing the normal evolution of a spent fuel repository for the TILA-99 performance assessment study in Finland. He is currently managing a performance assessment for low-level waste disposal in the UK.

Dr. Roger Wilmot

Dr. Roger D. Wilmot is a Senior Consultant at Galson Sciences Ltd. He has degrees in Earth Sciences from Cambridge University (BA) and Imperial College, London (PhD). He is a geologist with over 20 years experience in providing a broad range of research, consultancy and management services to a range of clients. This involvement has included a review of validation in the context of radioactive waste disposal, and the development of guidance concerning the treatment of validation in safety cases. On behalf of Her Majesty's Inspectorate of Pollution and the Environment Agency, he has organised international seminars on "Validation," "Risk Perception and Communication," "Management of Safety Assessments" and "Use of the Expectation Value of Risk." He has recently completed a project on the use of the expectation value of risk, and contributed to a technical and policy review of the HMIP radioactive waste research programme. He has contributed to the development and use of computer codes for incorporating long-term environmental change into safety assessments. Recent work outside the UK has included descriptions of climatic and geomorphological evolution in Finland for POSIVA, a leading role in describing elements of a regulatory strategy for consideration of future human actions in assessments for SKI, and involvement in performance assessment and near-field systems analysis for the WIPP site in the US. He is currently managing an options appraisal for low-level waste management in the UK. Finally, he has experience of several QA programmes, and is the Company's Quality Assurance Manager.

Evaluation of SKB's Report "Deep Repository for Spent Nuclear Fuel: SR 97 – Post-closure Safety", Focusing on the Assessment of Transport Processes in the Geosphere

Anders Wörman and Shulan Xu

Department of Geoscience
Uppsala University
Villavägen 16
S-752 36 Uppsala, Sweden

June 6, 2000

Abstract

This report describes a critical review of the safety assessment performed on the final repository for nuclear waste in Sweden that is proposed by SKB in "Deep Repository for Spent Nuclear Fuel: SR 97 – Post-closure Safety". The review was requested by the Swedish Nuclear Power Inspectorate (SKI).

The waste repository consists of several barriers that work together with the purpose of delaying radionuclide migration and reducing the activity that eventually affects the biosphere. A main criticism is the lack of a formal risk analysis and uncertainties in several analyses that make it difficult to comprehend the overall risk of the repository. A formal risk analysis should comprise a probabilistic treatment of all components included in the system. This is not the case in the SKB's report since the probabilistic analyses are limited only to certain aspects. The use of conservative model parameters are not a substitute for risk analysis nor can they compensate for possible model biases. Bias can be expected in most of the existing models of radionuclide migration in fractured bedrock.

SKB should present a clear comparison on the importance of the different barrier components (uranium-dioxide matrix, copper canister, buffer and bedrock) on the retardation of radionuclides. It is unclear as to what extent the capacity of the bedrock to retain migrating radionuclides is critical to the capacity of the repository. A large part of the SR 97 report is focused on retardation processes in bedrock and a reader can interpret this as the technical weight given on retardation in the bedrock. However, with the present state of knowledge, it is our opinion that we cannot with an acceptable degree of accuracy predict the radionuclide transport in bedrock or quantify risk levels associated with radioactivity in the biosphere. There are large uncertainties concerning the way by which sorption processes should be formulated and the impact of colloids on the transport that can be absolutely decisive in a long-term perspective. In the SKB report, the buffer erosion is treated in an arbitrary manner which can have an effect on the release rate of radionuclides and the form in which they are released (dissolved vs. particulate fractions). Also the matrix depth that is available for diffusion in the rock is not well known and this circumstance alone contributes to a large uncertainty in the prediction of radionuclide migration over very long time periods.

Due to the lack of understanding of radionuclide migration in crystalline rock, the reliability of the nuclear waste repository depends to a large extent on the engineered, local barriers, i.e. the uranium-dioxide matrix, the copper canister and to some extent the bentonite buffer zone. However, the report does not clearly cover conceptual uncertainties or other types (parameters, scenarios) of uncertainties in the modelling of the dissolution of the uranium-dioxide matrix. Furthermore, there is no technical or scientific rationale presented for the selected rate by which the copper canisters are broken. These deficiencies in the analysis implies that the presented breakthrough curves in the biosphere for different radionuclides are difficult to interpret in terms of 'risk levels' and, therefore, have a limited value.

Contents

1. Background and Structure

This report is a review of the Swedish Nuclear Fuel and Waste Management Co's (SKB) final disposal strategy for high level nuclear waste, as described in "Deep Repository for Spent Nuclear Fuel: SR 97 – Post-closure Safety". The review was conducted on behalf of the Swedish Nuclear Power Inspectorate (SKI), Department of Nuclear Waste. SKB's report comprises a technical description and safety assessment of the repository for spent nuclear fuel that is planned to be located at a depth of 500 meters at a suitable site in the Swedish bedrock. The risk analysis takes various future scenarios into account, with respect to hydrology, climatology and geological evolution and covers aspects of a number of different biogeochemical processes. Statistical methods have been used to treat uncertainties in existing data and scenarios. Safety assessment is a comprehensive and difficult undertaking where many aspects of uncertainties are to be balanced against each other with the aim of assessing the total safety of the repository. However, this review has been limited to focusing primarily on the analysis of radionuclide transport through the geosphere in the event of a complete or partial failure of the local barrier functions. Transport in the geosphere (pp. 270 – 330, Volume II of the Main Report) is mainly dealt with although the importance of transport in the geosphere relative to the local barrier system and dispersal processes in the biosphere are also investigated.

Firstly, general comments are presented on the risk analysis, focusing on the primary functions of the repository and the way in which the properties of the geosphere have been taken into account in repository safety. The discussion continues with the calculation of radionuclide transport through the geosphere to the biosphere. A main point is the difficulties of coupling, in a transport calculation, the chain of media, the engineered/local barrier, the geosphere and the biosphere, that affect the target variables established (radioactivity or radiation dose per year in peat mosses).

Finally, a more specific criticism of the transport calculations for radionuclides in fractured rock is presented.

2. General Comments on the SR 97 Safety Assessment and on SKB's Final Disposal Strategy for High Level Waste

According to SKB, the waste management method proposed in SR 97 can be justified on the basis that the radioactive waste is isolated by engineered barriers from any contact with the ecosystems that are necessary for human life. Radionuclides that accidentally are released from the repository are retarded physico-chemical processes in the geosphere, which results in a change in isotope composition through radioactive decay and a reduction in the total activity due to dilution. However, the report does not clearly describe how different repository functions interact and it does not clearly describe their relationship to the safety assessment, which is one of the purposes of SR 97. It is an essential pedagogical matter to clearly explain the basic functions of the repository concept and the risk of each function. More specific criticism of the safety assessment is summarized in the five points below:

1. *The lack of a formal risk analysis can be viewed as a methodological deficiency*

On page 444, it is stated that the report does not include a formal risk analysis or methodological analysis of the probabilities that can be associated with various scenarios for radionuclide release (possible FEP's) or combinations of scenarios. Although there are considerable problems connected with a formal risk analysis, this question is of overriding interest and should be the focus of considerable methodological developments. One basic problem now is how to evaluate risk levels without detailed knowledge about how the safety assessment has been performed.

2. Selection of conservative parameter values cannot generally compensate for possible errors in models

On page 292, SKB makes a general observation concerning models – that confidence in models must be on a par with the decisions influenced by the model predictions. One area where confidence in the models is relatively low is the retardation of radionuclides in the geosphere (see below). An indication of this is the wide range of physical and chemical parameter values that is found both in site characterisations and laboratory experiment with rock. SKB argues that deficiencies in the representation of processes and lack of knowledge of parameter values can be compensated for by selecting "conservative" values for parameters. However, SKB does not state exactly how this must be done, which can only be viewed as a methodological deficiency. On several occasions, it is proposed that "pessimistic" parameter values should be used. However, pessimistic values cannot simply compensate for errors in the empirical relationships that define the parameters.

3. Unclear justifications for selected combinations of uncertainties in the scenario analyses

The release analyses reported on pages 300 – 312 and the description of the risk analysis provided on pages 313 – 317 are based on certain basic assumptions concerning clearly delimited scenarios covering the performance of the local barriers in terms of resistance to mechanical influences, erosion of the buffer, corrosion, fuel matrix solubility limitations inside the canister etc. It is unclear in which way uncertainties are combined as well as how certain uncertainties are limited. Uncertainties in modelling concepts are described in greater detail in Section 4.

4. The geosphere is accorded a large degree of significance in the analysis of uncertainties

One way of characterizing the repository and differentiating a risk analysis is to focus on three typical times: 1) the time taken before a single canister starts to leak 2) the time taken for the entire radionuclide inventory of the repository to be released (release time) and 3) the residence time for radionuclides in the geosphere. It seems that SKB assumes that the first two times can be well defined or, at least, are not subject to probabilistic calculations. The main uncertainties are introduced in the determination of the residence time for radionuclides in the geosphere. However, an extended release time (defined here as the sum of times 1) and 2) is absolutely necessary to ensure that the maximum concentrations in the biosphere, shown in Figures 9.29 to 9.40, are below appropriate limits. The retention of transported radionuclides in the geosphere is important for evening out the radioactive flux to the biosphere over time which contributes to a reduced radiation dose per time (if there is a low accumulation in the ecosystem). However, the typical times of 1) and

2) are of decisive importance for the performance of the repository. In particular, considerable uncertainty can be expected due to conceptual errors in the modelling of corrosion, erosion, solubility and chemical evolution in combination with changes in the external conditions. These uncertainties are not clearly taken into account in the overall risk assessment.

5. The importance of conceptual errors in models can be analysed to an greater extent

Conceptual errors in models may imply considerable uncertainty with respect to local barrier performance calculations. Therefore, it is particularly important to ensure that the analysis of the barrier functions is combined with a formal risk analysis as well as with a sensitivity analysis of the assumptions used in modelling. A list of critical assumptions should be prepared and basic analyses of the importance of simplifications should be conducted. Comments on critical modelling assumptions about retention in the geosphere are provided in Sections 3 and 4 of this review report.

A decisive factor in the release calculations reported on pages 300 – 317 is the solubility of the uranium-dioxide matrix. According to SKB's report, the intensity with which the radionuclides are released is dependent upon the solubility of the uranium-dioxide matrix (page 289) and the solubility limitations in the environment of the uranium matrix. The details of how the calculations of all of these processes and their scenarios have been combined have not been reviewed here. However, there is no doubt that this determines the maximum doses in the biosphere. In principle, it is possible that certain combinations of changes in solubility models or parameter values can lead to considerable changes in the results. Furthermore, considering the fact that the repository will comprise a number of canisters, the distribution of times for the onset of radionuclide release will be an important factor. In this respect, the assumptions used in the scenarios are of decisive importance (canister defects and canister failure).

6. The repository design is not based on an engineered planning of radionuclide release

The repository design does not appear to be engineered so as to ensure that that an extended release process and dilution will be achieved. Similar ideas about ensuring a controlled release process have previously been presented in the high radioactive waste management community, and it is unclear why these have been rejected. The final disposal strategy seems to now focus on the isolation of the waste for a long time regardless of whether this results in a sudden and simultaneous degradation of the local barriers in a remote future. It is important, from a pedagogical and safety-related standpoint to justify the proposed design.

3. Calculation of Radionuclide Transport through the Geosphere to the Biosphere

In one of the scenarios included in SKB's risk analysis, it is assumed that canister failure and the release of radionuclides through the bentonite buffer and surrounding rock will occur. One major difficulty in determining the effect of the retention of released radionuclides is our deficient knowledge of matrix diffusion and sorption. Based on assumptions concerning model characteristics for matrix diffusion, diametrically opposing results can be obtained. The calculated time for a radionuclide to be transported 500 meters in the groundwater can vary from a few years to several hundred thousand

years, depending on the model selected (see the next section). This uncertainty is aggravated by our deficient knowledge of the variability of sorption mechanisms in time and space, erosion of the bentonite buffer and the occurrence of "natural colloids" in the groundwater over the next thousand to hundred thousand years. Furthermore, we know from isotope studies that the residence time probability density function for water in the groundwater can also be very wide as a result of the different transport paths (Rodhe and Killingtveit, 1997). The expected residence time for water that flows pass the a repository can be viewed as markedly uncertain.

With the current level of knowledge of basic reactions and the natural variability of the groundwater flow as well as the reactions, it is therefore difficult to determine with a reasonable degree of certainty, the expected transit times for radionuclides in the groundwater in the event of a canister failure. This deficiency in the knowledge of basic processes and the natural variabilities is difficult to translate into a probability density function for transit times. Therefore, with the present level of knowledge, we should be careful with according radionuclide retention in the rock a decisive importance for repository performance. In some of the cases reported in Figures 9-28 to 9-40, the residence time for nuclides in the geosphere is significant relative to the time before the onset of radionuclide release (as a rule 200,000 years). For example, the calculation case in Figure 9-28 shows that the average residence time of Se-79 is at least 100,000 years (approx. phase shift between initiation and maximum concentration) while the residence time for I-129 is considerably shorter. Bearing in mind our deficient knowledge of matrix diffusion, sorption and groundwater flow, there are uncertainties in these retention times that are of the order of magnitude of 100 – 1,000 times (see Section 4).

Another question that is of utmost important for the calculation of radionuclide transport concerns the treatment of the biosphere as a boundary condition vis à vis the geosphere in terms of hydrology and biogeochemistry. It is not stated clearly how the accumulation of radionuclides in the peat mosses, which is now used as a main environmental impact variable, is taken into account. In other words, to what extent is it expected that the radionuclides that reach the peat mosses at an early stage in the release sequence will accumulate there until a later time in the release sequence? The assumptions concerning dispersal processes in the biosphere are of decisive importance in the calculation of the activity in the peat mosses. The descriptions on pages 281 to 284 are not very clear on this point and this review does not deal with the ecosystem modelling.

4. Comments on the Retention Process Model

Detailed comments on SKB's way of calculating the transport of radionuclides in the geosphere are presented in this section.

Surface Diffusion and Sorption Kinetics

On page 271, section 9.9.3, SKB states that surface diffusion could be a possible cause of the particularly high diffusivities in the rock matrix. However, it is possible that the neglect of sorption kinetics is another reason for the misinterpretation of experiments where diffusion occurs in the rock. Sorption kinetics in the rock matrix can, under certain conditions, lead to higher concentrations in a breakthrough curve for a pulse that advects in a rock fracture (Xu and Wörman, 1999). It is not trivial to assume conservative values for distribution coefficients that compensate for this effect.

On page 272, SKB states that it has selected pessimistic values "within the uncertainty interval" for K_d. This approach has not been clearly explained. In particular, it is not clear why these pessimistic values could compensate for the neglect of sorption kinetics, surface diffusion or other deficiencies in the process description. The pessimistic K_d values represent disadvantageous equilibrium chemical conditions and do not necessary result in a "general" compensation for various errors in the transport model.

Colloids

SKB states, on page 293, that the concentrations of colloids found in the groundwater are so low that they can be neglected in the modelling of radionuclide migration in Swedish bedrock. It is unclear how this conclusion has been reached. On page 279, SKB refers to the study conducted by Allard et al (1991) that shows that the natural occurrence of colloids is low in Swedish groundwater at relevant rock depths. Other references are not given.

The issue is complicated by the fact that the composition of the groundwater could change over the next 100,000 years and vary considerably at different locations in Sweden. Erosion of the buffer – which can result in local colloid production - is discussed below. Furthermore, natural variations in colloid concentration can occur in connection with changes in hydrological conditions with changing glacial conditions and altitudes. The travel time for water is approximately 1,000 years (page 278) to the repository depth which means that colloid particles produced in the biosphere could reach the repository within the times that are relevant in a risk analysis.

Most investigations of natural fractures indicate a significant presence of gauge material that adheres on the fracture walls. Sufficiently fine grained gauge particles could be diffused in the water depending on the balance between cohesive and diffusive forces that may change over time.

The method of studying the effect of colloids on radionuclide transport, which is described on page 280, is unclear. The effect of colloids is introduced by reducing the K_d value for radionuclide sorption in the rock matrix. This method is questionable and the sorption affinity that radionuclides actually have to colloid particles is also questionable (this has presumably never been methodically investigated). The occurrence of colloid particles would also entail a further speciation of radionuclides in the rock fracture water in a particulate phase and a true soluble phase. The particulate phase would probably largely be prevented from diffusing into the rock matrix (due to mechanical filtering) and therefore has a higher mobility. This results in a lower concentration of radionuclides in the rock matrix, although no essential change in the K_d value in the rock matrix (if a linear adsorption isotherm is assumed). A fictitious reduction in the K_d value would also result in an increase in mobility, although this would be in an "undefined" manner which cannot be considered to be adequately supported by scientific evidence.

Erosion of the Bentonite Buffer

In SKB's report, it is assumed that colloid transport can be neglected since bentonite release is considered to be too small with respect to certain experiments that focus exclusively on erosion. However, it seems as though SKB assumes that erosion is of no significance to the release of radionuclides and to the release time mentioned above.

It is possible that there could be two mechanisms leading to radionuclide transfer from the outer surface of the bentonite buffer to the surrounding groundwater: molecular and advection through the erosion of the buffer. The erosion leads to the release of a mixture of colloidal material and radionuclides (in the buffer pore water and sorbed onto the solid surfaces of the buffer) in the surrounding groundwater. One question is whether erosion can be considered to be small with respect to the radionuclide release (in comparison with molecular diffusion). Another question is whether the dilution of the bentonite particles is so high that sorption to the colloid bentonite particles can be neglected. Since the K_d value decreases with a decrease in particle concentration, the assumption in the report, that the impact of colloid particles is low, could very well be correct. However, the particle concentration from the bentonite buffer should be added to the natural particle concentration in the groundwater.

It is questionable whether the extent of the erosion can be determined by experiment. Erosion is mainly dependent on the flow rate (actually the shearing stress between the water and the bentonite buffer) and the properties of the buffer. Since the flow rates can vary within a very large interval depending on the heterogeneity of the rock, there should be considerable uncertainty in this question. It can be expected that erosion is of greatest importance in those cases where the highest shear stresses occur.

The erosion mechanisms should be set in a risk analytical context that can clarify its overall significance. The probabilistic flow calculations (such as those presented on pp. 273 – 274) that are mainly presented in the report do not include an analysis of local flow rates or shearing stresses. This means that the assessment of erosion is uncertain.

Matrix Diffusion

On page 278, a relationship is presented for the travel time of radionuclides in fractured rock. The relationship is based on a model for matrix diffusion that assumes an infinite penetration depth. This contradicts the assumptions of a limited penetration depth described on the previous page, which is also indicated in the text. However, the main problem is that the choice of model makes a significance difference for predictions.

If a limited penetration depth is assumed, under certain additional assumptions, it can be shown that the residence time can be described as follows (Xu and Wörman, 1999).

$$t_{transport} = t_w + F L \varepsilon_p \qquad (1)$$

where L = the maximum penetration depth [m] (e.g. half of the distance between two fractures), ε_p = matrix porosity, $t_w = x/U$ [s], $F = a_w\, x/q_0$, x = distance [m], U = flow rate in cracks [m/s], a_w = specific surface area [m^2/m^3] (surface area per volume of water) and q_0 = specific flow [m/s]. If the element is sorbing (radionuclide), the expression for the transit time will be $t_w + F L \varepsilon_p (1+(\rho / \varepsilon_p) K_d)$. The conclusion with respect to residence time will be completely different compared to that reached using the expression provided in the report. The equation on page 277 of SR 97 is as follows:

$$t_{transport} = t_w + F^2 D_e \varepsilon_p \qquad (2)$$

where D_e is the diffusivity of radionuclides in the rock taking tortuosity and constrictivity into account.

Assuming that t_w is small (namely that retention is significant) the ratio between $t_{transport}$ according to (2) and (1) will be $(F\ D_e)/L$. If the calculation example described on p. 277 of SR 97 is applied, where F = 250 000 year/m and $D_e = 3x10^{-6}$ m^2/year , the product $F\ D_e$ can be estimated at about 0.75. On page 276, it is assumed that the maximum penetration depth is between 2 and 20 meters, which means that the estimated residence time in SKB's report is up to 25 times shorter than that obtained using (1). Therefore, greater knowledge of the maximum penetration depth is important to an assessment of the impact of the matrix diffusion on radionuclide transport.

Studies of the microstructure in granite and historical evidence of the matrix diffusion indicate that the diffusion is limited to a relatively narrow zone close to the fracture surface (Heath et al., 1992; Montoto, 1996). Observations of concentration profiles of the uranium series isotopes show that the penetration depth appears to be limited to a few millimeters or tens of millimeters. The higher matrix diffusion along the fracture surface is partially due to a higher porosity caused by stress relaxation and weathering processes. The pore volume available for transport decreases with an increase in depth due to intergranular bonding and mineralization products. Diffusion experiments conducted by Johansson (2000) show a clear reduction in the diffusion coefficient with the thickness of the specimens.

If it is assumed that the maximum penetration depth is 10 mm instead of 20 meters, the residence time, according to (2) will be about 100 longer than that predicted by (1). Figure 1 shows penetration curves using different assumptions for maximum penetration depth for a constant boundary concentration. All parameter values are taken in accordance with section 9.9.7 of SKB's report: $a_w = 1000\ m^{-1}$, x = 500 m, $D_e = 3x10^{-6}$ m^2/year and $q = 2x10^{-3}$ m/year. These values can be converted into a fracture aperture = 2 mm and a flow rate in a rock fracture of 1 m/year (assuming a fracture frequency of 1 per m). Since the concentration at x=0 is kept constant, the concentration at x=500 m approaches this value with an increase in time. We can see that 90% of the final concentration is obtained after time $t_{90\%}$ = 830 years when the maximum diffusion depth is L=10 mm, t=11,000 years when L=2 and 150,000 years when the penetration depth is more than 20 meters. The total difference in $t_{90\%}$ (200 times) is of decisive importance for the assessment of the impact of the matrix diffusion on the retention of radionuclides in the geosphere. The difference decreases with an increase in sorption affinity within the interval $0.01 < L < \infty$ since the effective diffusivity decreases. In spite of this, realistic measures of the maximum penetration depth are important for the results presented in diagrammatic form on pp. 303 to 320.

SKB should clearly discuss how it intends to treat and technically evaluate such conceptual differences in model concepts that can result in essential differences in conclusions concerning radionuclide transport processes. As with the strategy reported for flow modelling, several different model concepts should be used to describe retention processes (to represent uncertainties in our way of understanding and mathematically describing these processes).

This uncertainty is discussed in the calculation of residence times on p. 278. The conclusion proposes that the travel times for water should be given as t_w. This does not alter the fact that the determination of the radionuclide travel time will still be affected by how the matrix diffusion is quantified. The transport calculation is briefly described on pages 291 and 295 under the heading, FARF31, where SKB states that the matrix diffusion is taken into account as a radionuclide retention process but does not state exactly which model assumptions are made.

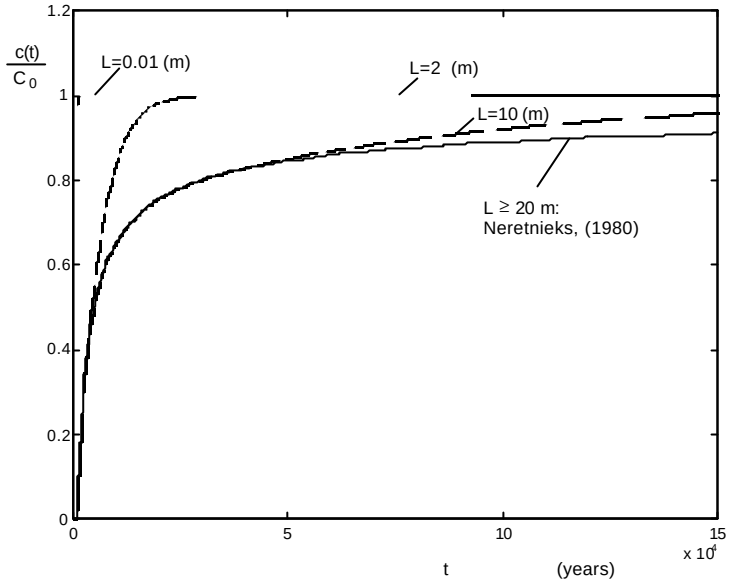

Fig. 1 Breakthrough curves at x = 500 m for the migration of a non-sorbing element due to a constant concentration at x = 0 and zero initial concentration. All of the parameter values have been taken from SKB's report and are described in the text.

Data and Empirical Studies

As described in the section above, the residence time for radionuclides in the geosphere is related to two terms expressing the residence time for water and the impact of matrix diffusion as well as sorption, (1) and (2). In order for radionuclide retardation to be significant in this context, the other term (1) or (2), that expresses matrix diffusion and sorption, must dominate. The main focus of empirical studies should therefore be placed on defining relationships that determine matrix diffusion and sorption. Since there is a correlation between the properties of the water pathways (fractures) and matrix processes, the flow field cannot be neglected. This is expressed in (1) and (2) by the fact that the F-factor represents the specific flow.

The F-factor is defined as (a_w x/q_0), where a_w is a specific wet surface ("wetted" surface), x is the distance and q_0 the specific flow. However, it should be remembered that (1) and (2) are based on assumptions of how the processes are to be described and how the residence times are to be defined. Essential questions relate to the description of the processes and the resulting definition of parameters. For example, it is important to improve the data describing the variation of tortuosity, constrictivity and porosity with distance from the fracture surfaces. This information is decisive for an improvement of our understanding of matrix diffusion and sorption. Bearing in mind that different models can involve a difference in the estimated residence time for radionuclides on the order of several orders of magnitude (see above) greater understanding is necessary. Unfortunately, there is a lack of data in the report describing the matrix structure around fracture surfaces.

The confidence level for data which are important to a determination of the flow field at the investigated sites can probably be assessed as good. Bearing in mind the fact that both discrete network models and continuum models give similar results (p. 293) and the fact that a stochastic approach has been used (where uncertainties can be quantified in a relatively credible manner), it is

possible to assess the data and the interpretation of hydrological data as good. This conclusion is also reached in the report. However, there should be premises for using data to study correlations between a_w and q_0, which are essential to radionuclide retention (Table 9-3, p. 298). It is unclear whether the correlation has been evaluated, even if this is described as a potentially important part of the analysis on p. 298.

References

Xu, S., Wörman, A., 1999. "Implications of Sorption Kinetics to Radionuclide Migration in Fractured Rock", Water Resources Research, 35(11), 3429-3440.

Heath, M.J., Montoto, M., 1996, Rock Matrix Diffusion as Mechanism for Radionuclide Retardation: Natural Radio-Elements Migration in Relation to the Microfractography and Petrophysics of Fractured Crystalline Rock, Report EUR 17121, European Commission, ISBN 92-827-3907-4.

Heath, M. J., Montoto, M., Rodriguez Rey, A., Ruiz de Argandona, V. G. and Menendez, B., 1992. Rock Matrix Diffusion as a Mechanism of Radionuclide Retardation: A Natrural Analogue Study of EI Berrocal Granite, Spain. Radiochimica Acta 58/59, 379-384.

Johansson, H., 2000. "Retardation of Tracers in Crystalline Rock: Sorption and Matrix Diffusion of Alkali Metal and Alkaline Earth Metal Tracers in Laboratory and Field Experiments". Doctoral thesis. Chalmers University of Technology, Gothenburg, Sweden, ISBN 91-7197-893-3.

Rodhe, A. Killingtveit, Å, 1997. "Catchment hydrology", In Geochemical processes, weathering and groundwater recharge in catchments, A.A. Balkema, Rotterdam, Eds:Saether, O.M. & de Caritat, P., pp 77-107.

Biography

Anders Wörman is Associate Professor of Hydraulics at the Royal Institute of Technology, Stockholm (KTH), of Sedimentology at Uppsala University and is employed a Lecturer at the Department of Geoscience, Uppsala University where he is also Director of Studies. He obtained his MSc in civil engineering in 1985 in at KTH, Swedish "licenciate" degree in hydraulics in 1987 and PhD in hydraulics in 1991 at KTH. Between 1991-1993, he was employed as a consultant at Vattenfall Utveckling AB, Älvkarleby. From 1992-2000, he has been employed at Uppsala University and was appointed co-ordinator of a new MSc degree in Aquatic and Environmental Engineering at Uppsala University of Technology.

Anders Wörman's research profile includes mathematical, experimental and field methods for the analysis of transport processes in different aquatic environments such as water courses and fractured rock, involving both hydromechanics and environmental chemistry. He has been awarded a national scientific prize (Thernwall Prize 1992), initiated and led a number of research projects that have led to higher academic dissertations and published about 25 scientific articles in international journals. The research is financed by government agencies (SKI, STEM), trade organizations (Elforsk AB) and government research councils (Nutek, NFR, BFR).

Shulan Xu is completing his doctorate at the Department of Geoscience at Uppsala University. He took his degree in thermoengineering at Shanghai Institute of Mechanical Engineering, China and his Swedish "licenciat" degree in water treatment technology at KTH, Stockholm. Shulan Xu was employed as a consultant at Shanghai Marine Equipment Research Institute in Shanghai during 1979 – 1991. From 1995 to 2000 he has worked on a research project, financed by the Swedish Nuclear Power Inspectorate (SKI). The aim of the project is to study how the spatial variability in the rock's geochemical and physical properties affects radionuclide migration in individual fractures. He has published 7 scientific articles in international journals.

Review of SFL 3-5 Performance Assessment

Pierre D. Glynn

U.S.Geological Survey
Water Resources Division
432 National Center
Reston, Virginia 22092, USA.

My review focused on a careful reading of the main SFL3-5 report (SKB TR-99-28) with occasional referencing to supporting documents (Compilation of Data for the analysis of radionuclide transport: SKB R-99-13). I have highlighted what I believe to be the most important questions and issues.

Executive Summary:

p. ix, para. 2: Why aren't the sorption and diffusion data chosen by taking into account the rock/medium composition and factors such the amount of wetted surface area and the porosity? Certainly water composition should be important but so should the mineralogy of the rock/medium surfaces encountered and the amount of surface area encountered per volume of water. Taking straight "Kd" data expressed in m^3 per kg and determined for granite and applying it directly to gravel without even normalizing the numbers for the differences in wetted reactive surface areas does not sound reasonable. Certainly if this hasn't been done then it should be said why it wasn't judged important.

p. ix: what is the expected composition of the gas? Where is it expected to come from? What processes generate it?

Throughout the executive summary: Why is there no quantitative idea given of what the words "short term" and "long term", or "long life" mean?

p. xi, 4^{th} para.: I would argue that if the near-field barriers are built strongly enough, then you wouldn't have to worry about far-field conditions. The report generally gives the impression that SKB's near-field design will simply not hold up and that they are therefore overly dependent on the protection that they think will be afforded by the far-field barrier.

Chapter 1:

Just as there is no quantitative idea of time scales given, at least initially, the report also takes a long time before allowing the reader to get an idea of what SKB considers a "regional" scale flow model. From descriptions of the actual flow modeling conducted later on in the model, it appears that "regional" means something on the order of 10 km. For me that's almost "local" scale. Why didn't SKB consider more extensive "regional" models in their analysis?

Chapter 3:

p. 3-11: This is the first time that I have seen a gravel size fraction (4-32 mm) referred to as being made up of “small” particles. It is also the first time that I see somebody referring to the “large” surface areas of gravel particles. What does SKB consider to be “large” particles? How does SKB refer to the surface area of clay-size particles? Gravel is not known to have either "large" surface areas or particularly good sorption properties. SKB should cite external research that shows that gravel, of the type and composition that will be used, does indeed have considerable sorptive properties. The external research should be consist of peer-reviewed articles, preferably authored by scientists who are not consultants or employees of SKB. One of my impressions from the SFL3-5 performance assessment is that it often looks as though SKB selectively picks out just the data and conclusions that they want, ignoring other data and analyses that may offer very different conclusions and that may not fit SKB's preconceived engineering notions.

P. 3-11: SKB needs to clearly explain why they didn't want to use a bentonite barrier or other relatively impermeable barrier that would likely have a much higher sorption capacity.

p. 3-12: The report mentions "the SKB redox experiment". This was indeed an interesting, well-conducted, experiment. It did, however, have some limitations. First, the oxygenated water that was used, and also probably the relatively shallow fracture that was used, contained significant amounts of organic matter that was able, through the catalytic capabilities of microbiota, to rather rapidly reduce the dissolved oxygen that was introduced. This is not necessarily likely to occur under conditions that differ from present day conditions (e.g. under a warm-based ice-sheet), or in other types of fractures than the relatively wide, gouge-filled, fracture that was chosen. Which brings me to the second point which is that thinner fractures with less gouge material may behave quite differently in terms of the operative redox processes and particularly, in terms of the relative speeds of reaction of those processes (relative to ground-water flow).

Chapter 4:

p. 4-2: It is interesting to read here that SKB is worried about the "interactions" of the different materials used for a) the high-level waste repository and b) the low-and intermediate level repository. First, why don't they exactly say what "interactions" they are worried about?

Secondly, just a few pages earlier (p. 3-13) they mentioned the fact that they thought that "the buffering properties of the rock will keep the pH and Eh of the groundwater at repository level roughly unchanged". So why do they consider that they need at least 1 kilometer distance between the repositories? They just said that the rock provided a strong enough buffer that the local ground waters would essentially remain unchanged. Thirdly, and even more importantly, why is 1 km in the horizontal direction considered the minimum amount of buffer required when the repository is being built at only 300 m depth. If their argument about a minimum separation distance of 1 km is true, then it would seem to me that they really should place the repository at a minimum depth of at least 1 km, (and probably more since vertical flow may predominate during periods of glacial advance). The other interesting point is that SKB does not seem to take the hydraulic conductivity of the rock at the various sites into account when determining the appropriate minimum separation distance. That is probably not a bad idea. However, they should mention why they take this approach.

Chapter 5:

OK. I'm not qualified to judge the Biosphere section.

Chapter 6:

p. 6-2: The report states that the predicted temperature increase of 5 ^{o}C, caused by radioactive decay, is not significant for the performance of near-field barriers. Although I probably agree with that statement, does it also hold for the steel corrosion rate? That is, wouldn't the steel corrosion rate be increased? The often quoted rule of thumb is that reaction rates generally increase by a factor of 2 for every 10 ^{o}C increase. What would be the effect on the steel canister corrosion rate? SKB also needs to take the potential salinity of the waters into account when answering this question.

p. 6.3: Just because the reference scenario assumes that the "regional" groundwater conditions are stable, and that therefore no changes will "occur in either the direction or the size of the groundwater flow into the repository area", does not mean that the initial assumption is reasonable. What is the point of doing a performance assessment if potential changes and hydrologic, structural and geochemical conditions are not taken into account? I think SKB

needs their make their case for considering only "the reference scenario" much more strongly than they have done in the report.

p. 6-5: It is interesting to read that SKB projects that all organic material in the waste will be consumed after only 600 years and all the steel after only about 8000 years. What will be the remaining reductants left in the repository near field then after 8000 years? What quantities of these reductants does SKB estimate will be left of those reductants? What does SKB expect will happen to redox conditions in the near-field after 8000 years?

p. 6-7: The report says "The redox potential, pH and salinity of the water, and its content of complexing agents and colloids, are of great importance for the performance of the near-field barriers and for the migration of radionuclides and other solutes". What is then the justification for ignoring the full extent of possible temporal changes in those properties throughout the performance assessment?

p. 6-10: I note in table 6-1 that the chlorinity of the "saline" water used is only 181 mmol/L, which translates to about 6000 mg/L Cl. If seawater intrusion occurs (rather than Baltic water intrusion), the actual chlorinity of that seawater is likely to be 3 times higher, about 19000 mg/L. Of course if deep brines were to flow through the repository, their chlorinity would be even higher. Hole KLX02 has a chlorinity of 45000 at only 1.7 km depth near Aberg. What maximum chlorinity (or salinity) would SKB actually consider in an actual performance assessment?

p. 6-12: The report states again that the composition of the waters has a greater effect on sorption properties than the composition of the materials. To me that is not obvious at all. First of all, different materials are likely to have different specific surface areas. Secondly, different materials simply have vastly different sorption capacities. For example, smectite minerals have cation exchange capacities which are hundreds of times higher than those of kaolinite or illite. Different materials also have different behaviors with pH, or at least different pH transition points at which the surface may change from being positively charged to being negatively charged. So what is the justification for considering water composition effects but not the effects of mineral composition or solid-surface area on sorption?

bottom of p. 6-16: The report states that the gravel fill is assumed to have sorption properties typical for Swedish rock. Did SKB normalize the Kd's taking into account the differences in surface to volume ratios between gravel and "Swedish granite"?

bottom of p. 6-17: The report does not discuss at all the uncertainties on the assumed rate of metal corrosion. What are the uncertainty estimates for the rates of corrosion?

p. 6-22: It would be nice if the report gave an estimate of the retardation factors applicable to various isotopes, but maybe that is coming later on.

p. 7-1: Why didn't SKB at least discuss their assumption of constant flow directions and flow intensity? How reasonable do they think it is?

p. 7-3: The report states: "The specific flow is greatest if the regional flow is directed along the tunnel. The flow is smallest if the regional flow is directed perpendicular to the tunnel. The same applies to the total flow in the tunnel." Can SKB explain this statement? Intuitively, I don't think it's correct.

p. 7-6, 3rd paragraph from the bottom: Why would it be difficult to put in a low permeability barrier, at least 10 times less permeable than the rock, at a site like Aberg? Maybe it would be difficult at the other two sites, because of their supposedly much lower hydraulic conductivities, but I don't see why it would be a problem at Aberg. And even at the two other sites, I believe that if SKB had spent has much effort drilling boreholes and collecting various types of data as they did at Aberg, they would probably find that the applicable hydraulic conductivities are probably much higher than those cited in the SFL3-5 report.

p. 7-7, 2nd para.: How reasonable is it to assume horizontal flow in areas of regional groundwater discharge, such as at Aberg and Beberg?

p. 7-7, section 7.3.6: "The results show that in such a rock mass, the heterogeneity leads to an increase of the total flow in SFL 4 by a factor of about 2". Don't the results depend on the statistical properties used to define the stochastic continuum model? How sensitive are the results to uncertainties in that definition?

p. 7-8, bottom: Does the report actually imply that the Aberg is in a regional recharge area? That's news to me. (i.e. it states that the mean direction of flow is 30 degrees downward at Aberg). Also how does SKB use this result to state a little later (bottom of p. 7-12) that the flow at repository depth is largely horizontal? 30 degrees down is nowhere near horizontal in my book.

bottom of p 7-13: Given the very different hydraulic conductivities for the 3 different sites why didn't SKB adapt their backfill strategy individually to each of the 3 different sites. That is,

why didn't they pick a different strategy in particular for Aberg, with a low-permeability fill instead of a gravel fill?

General comment on flow modeling: Because of the relative paucity of data from Beberg and Ceberg, an equivalent homogenous porous medium was assumed in the flow models of the 2 sites. In contrast, because much more data was available for Aberg, a stochastic continuum model was used. Although I can understand why this was done, this approach does contain an element of illogic. If we assume that indeed the rock at Ceberg is much less fractured than at Aberg, it would stand to reason that the heterogeneities that do exist would actually influence ground-water flow to a much greater extent than at Aberg where the rock is supposedly much more extensively fractured. Therefore, why shouldn't one make the argument that actually an equivalent porous medium model would actually be much more suitable for the Aberg site than for the Ceberg site?

Chapter 8:

p. 8-2: Isn't the assumption that the properties of the concrete moulds and enclosures won't change with time a fairly big assumption? Why is this assumption justified?

p. bottom of 8-3: the report states that the SFL3 tunnel has a concrete plug at both ends and that therefore released radionuclides will only be able to leave by the rock. What are the assurances that the concrete won't crack over time? And if this doesn't matter, then why not?

p. 8-10, first para.: I haven't read Carbol and Engvist (1997). Why is it reasonable to assume that the same sorption data can be used on both granite and gravel? (see my earlier comment).

bottom of p. 8-10: Again. What are the uncertainties related to the corrosion rates of steel and zircaloy? This is a pretty big issue since it controls the release of several radioactive isotopes (including ^{93}Mo, one of the isotopes of concern).

p. 8-11, table 8-3: How come distribution coefficients are not provided for saline water in concrete? Are they deemed unimportant? Why?

p. 8-13: Given the big difference in the results obtained for the "saline" water case (compared to the low salinity case), I would think that it would be very important for SKB to consider the possibility that waters of even higher salinity (seawater or shield brines) might intrude through the repository. Given the strong effect of water composition on radionuclide

sorption and retardation why didn't SKB consider the potential for intrusion of waters of even higher salinity?

p. 8-18: Aren't the matrix diffusion calculations rather overoptimistic? The Swiss and the Spaniards typically assume that the maximum penetration depth for matrix diffusion is at most 10 cm, and they usually use 5 cm in their calculations. Here SKB is assuming 200 cm in two cases (Aberg and Beberg) and 2000 cm in the other (Ceberg). I was told that the rationale for this is that those distances represent the 1/2 of the maximum separation between fractures at the 3 sites. Actually, I have seen several studies, by Montoto and others for example (see references in Glynn and Voss, 1999, SKI report, part II) that show that matrix diffusion is only likely to occur in a thin skin close to the fracture walls. This skin has significant microfracturing because of the stress release offered by the presence of the fracture and therefore offers a reservoir for matrix diffusion. As one moves away from the fracture, however, the amount of microfracturing decreases significantly and matrix diffusivities are likely to be insignificant. I was also told second-hand that the actual penetration depths picked would supposedly not matter in the final results. If that was the case, then why were such large maximum penetration depths picked?

p. 8-20: How does SKB reconcile the average advective travel time of about 900 years estimated from their calculations for Ceberg (Gideå) with the earlier SKB (SKB TR 91-28) report by Itnner and others (1991) that documents the arrival of 3 different radionuclide spikes arising from the Chernobyl accident in a packed borehole section at 97-106 m depth at the Gideå site after only 1 to 2 years? For reference, the radionuclide spikes arrived with different degrees of retardation, 263 days for ^{206}Ru spike, 516 days for the ^{137}Cs spike and 599 days for the ^{60}Co spike. Had this occurred because of inter-borehole leakage one would have expected that the isotope spikes would arrive simultaneously. My conclusion is that the calculated mean arrival time and flow model for Ceberg are not consistent with the available field evidence. Unless of course SKB now discredits their earlier work? In which case, they should formally state their reasons for doing so and formally publish any corrections.

p. 8-18 and 8-21: Why is a much higher flow wetted surface area assumed for Beberg than for the other sites? Is it just an arbitrary number picked just to be different?

p. 8-30 and 8-31: the report says that 3 ice ages are projected to occur during the 100000 years but that after that the "future evolution of the environment is uncertain". If that's the case, i.e.

the implication is that the occurrence of the 3 ice ages is then rather certain, why did SKB simply ignore any of their potential effects throughout their performance assessment? Here they refer to discussions in section 9.2, but actually there is just about no real discussion of this in that section. Isn't it rather strange to gray out the area after 100000 years on figure 8-10 because of the lingering uncertainty of climate evolution after that time? By the way, fig. 8-10 has the comparison and background levels switched.

General comment: I would have liked to see some assessment of the chemotoxic effects of Pu and U release. I didn't see any. Is this because the chemotoxic effects of Pu and U can be considered truly insignificant given their release concentrations?

p. 8-35: What are the "comparison levels" for the chemotoxic pollutants? How are they determined?

p. 8-35, last paragraph: SKB claims that chemotoxic concentrations will exceed the comparison levels sometime between 100000 and 10 million years in the future, but that this can be ignored because several ice ages will have come and gone and essentially the entire ecosystems will have been scraped away several times. I don't dispute this argument. However, it appears that SKB is selectively considering the probability of future glaciations when it suits them but ignoring it (in the case of radioactive releases) when it doesn't suit them. At a minimum, this is a rather inconsistent consideration of glaciations in the performance assessment.

Chapter 9:

p. 9-4, below fig. 9-1: The report states that when a continental ice sheet moves over an area, high water pressures underneath the melting area can lead to widening of fractures resulting in increased permeability. Although I don't disagree with this statement, I believe that there are a lot more uncertainties about the effects of ice loading on ground water flow, fracture widening/narrowing and hydraulic conductivities in the vertical and horizontal directions than the report lets on here. At least that was the impression I got from the presentations of Robert Muir-Wood and other geophysiscists at the glacial workshop in Hasselby a number of years ago. Has anything changed, i.e. has new knowledge emerged on this topic that allows SKB to so confidently predict what will happen? If so, why don't they cite the new work?

p. 9-5, first para.: The report cites Karlsson and others (1999) in stating that the penetration of oxygenated waters is not likely to affect the repository in any way because 1) of the great capacity of the metal and organic substances in the repository to reduce the oxygen and 2) because relatively few radionuclides in the waste will be affected by oxidation. Well, the report actually says earlier that all the metal and organic materials are likely to have been reduced away in the first 8000 years. So what happens in the next 92000 years when 3 glaciations are predicted to occur according to SKB? And what about the following 9.1 million years of relatively "uncertain" climate evolution that are being considered by the performance assessment. Also, certainly Pu and U speciation behavior and mobility can be expected to be affected by oxidation? So why is this insignificant? Finally, even if the direct effect on radionuclide speciation is insignificant, won't the corrosion rates of the steel and zircaloy be affected? What is the rationale for ignoring those effects on the performance assessment?

p. 9-5, section 9.3: What about the effect of earthquakes in "relatively unfractured" sites such as Gideå? I would expect that displacements there would be greater than at Aberg, because of the smaller number of potentially adjusting rock blocks. Is this wrong?

Final Comment:

This "performance assessment" report has 1) several logical flaws and 2) is not scientifically objective. There is a lot of good work done by individual SKB consultants. The problem is that the report does not consider all the available research that has been conducted, both by SKB consultants and by other scientists. The report only seems to select evidence/research pieces that fit preconceived notions supporting SKB's ultimate objectives. This is done rather poorly, which is why one can easily pick out inconsistencies and logical flaws.

The author

Dr. Pierre D. Glynn is a senior scientist for the U.S. Geological Survey, Water Resources Division, National Research Program in Reston, Virginia (1987 to present). He also serves as an associate editor for the journal Ground Water. Dr. Glynn's professsional training is in the areas of low-temperature geochemistry, isotopic geochemistry and ground-water flow and transport processes. He has a B.A. from Columbia University (1980), M.Sc. from University of Quebec in Montreal (1982), and Ph.D. from Waterloo University in Canada (1986). Dr. Glynn's present research interests concern: 1) the geochemical evolution of ground-water systems, 2) the reactive transport of contaminants in ground water, 3) radionuclide solubility and sorption modeling, 4) the thermodynamics of solid-solution aqueous-solution processes, and 5) ground-water dating with geochemical and isotopic techniques. In addition to conducting research, Dr. Glynn often teaches courses on ground-water geochemistry and transport processes. Dr. Glynn has been involved in conducting research on nuclear waste disposal issues since 1992, primarily for SKI, but also for the U.S. Department of Energy.

Comments on SKB's SFL 3-5 Preliminary Performance Assessment

Roger D. Wilmot
Mark B. Crawford

Galson Sciences Ltd
5 Grosvenor House, Melton Road
Oakham, Rutland, LE15 6AX, UK

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Contents

Summary

The Swedish Nuclear Fuel and Waste Management Company (SKB) has recently published a preliminary performance assessment (PA) for a disposal concept for long-lived low-level and intermediate-level radioactive waste (L/ILW). No decision has yet been made about the siting of the SFL 3-5 repository. For the purposes of the PA, SKB has assumed that the repository would be co-located with a repository for spent fuel (KBS-3 concept), and has therefore based the site characterisation data for the SFL 3-5 assessment on that used for the SR-97 assessment of the KBS-3 repository. Three hypothetical sites, known as Aberg, Beberg and Ceberg, have been used in both assessments.

This report presents a review of the SFL 3-5 PA undertaken by Galson Sciences Ltd on behalf of the Swedish Nuclear Power Inspectorate (SKI). The review examined all aspects of the PA, although particular emphasis was placed on the treatment of uncertainty, the use of probability, and the use of expert judgements. Limitations in the resources available for the review meant that it was restricted to the main PA report; the supporting documents were not reviewed.

Recently introduced regulations in Sweden have established an individual risk criterion for the long-term performance of repositories. The SFL 3-5 PA has not focussed on this criterion, but has been restricted to determinations of individual dose. Because the calculated doses are below the regulatory limit when the probability of significant events is effectively one, SKB has assumed that this approach is conservative and that event probabilities do not need to be determined. There is insufficient information available on the uncertainties in the PA to determine whether this approach is reasonable. The limited treatment of uncertainty also means that key sensitivities in system performance cannot be identified from the assessment results.

The SFL 3-5 PA is strongly reliant on the use of expert judgement. Judgements have been used to determine how the assessment should be conducted, and also to parameterise models in the absence of site characterisation data. The preliminary nature of the assessment means that the use of judgements is justified for both of these purposes. However, the PA documentation does not identify where judgements have been made or provide traceable links to the description, justification or review of individual judgements.

SKB defined four scenarios in the SFL 3-5 PA, but only used two of these as the basis for performance calculations – a Reference Scenario and a Future Human Actions Scenario. These scenarios are appropriate for a preliminary examination of the effects of hydrological and biosphere properties on individual doses, but the lack of a clear scenario development process limits the usefulness of the results in terms of overall system understanding. Also, the use of different biospheres at each site makes it difficult to assess the impact of different hydrological conditions on radionuclide transport in the far-field. The Future Human Actions Scenario does not consider intrusion or by-passing of system barriers, but is based solely on a change in dose conversion factors in the biosphere.

Overall, the SFL 3-5 PA is appropriate as a top-level document that summarises the assessment context, disposal system characteristics, key assumptions and results. A clearer treatment of uncertainties would help in developing an understanding of sensitivities, and the use of a Reference Biosphere at each site would help to clarify the significant differences between the sites in terms of long-term system performance.

1 Introduction

This report has been prepared by Galson Sciences Ltd (GSL) on behalf of the Swedish Nuclear Power Inspectorate (SKI) as part of SKI's overall review of the recently published SFL 3-5 performance assessment (PA) from the Swedish Nuclear Fuel and Waste Management Company (SKB) (SKB, 1999a). The SFL 3-5 PA is a preliminary assessment of a disposal concept for long-lived low-level and intermediate-level waste (L/ILW).

The SFL 3-5 PA is linked to the safety assessment of the KBS-3 disposal concept for spent nuclear fuel, also published recently by SKB (SR 97; SKB, 1999b). SR 97 compared long-term performance at three hypothetical sites (Aberg, Beberg and Ceberg), and the SFL 3-5 PA assumes that the L/ILW repository would be co-located with the spent fuel repository at one of these sites. Site characterisation and hydrogeological data derived for SR 97 are used as the basis for the SFL 3-5 assessment. GSL recently undertook a review of SR 97 on behalf of SKI (Wilmot and Crawford, 2000), and examined the use of probabilistic risk calculations and how expert judgements had been applied by SKB in the SR 97 assessment.

This report includes the same review objectives as GSL's review of SR 97, but the scope of the review has been extended to include a broader assessment of the overall approach to PA for SFL 3-5. The review addresses four principal issues:

- The methodology and scientific rationale that underlie SKB's approach to risk calculations.
- SKB's approach to defining calculation cases, including the role of conservative and realistic modelling.
- SKB's approach to the combination of distribution functions for PA input parameters, and SKB's approach to combining scenarios for overall safety assessment.
- SKB's approach to presentation and interpretation of risk results.

Section 2 of this report provides specific comments on the SFL 3-5 PA, presented according to the structure of the assessment report. Section 3 summarises these comments, and presents overall conclusions on the issues listed above. The review is focused on the main SFL 3-5 PA report (SKB Technical Report TR-99-28; SKB, 1999a). Supporting references (most notably Karlsson *et al.*, 1999; Pettersson *et al.*, *1*999; Skagius *et al.*, 1999a, 1999b) have been checked where cross-reference is made from the main report, but these references have not been reviewed in detail.

2 Specific Comments

In this Section of our review, we provide a commentary that follows the structure of the SFL 3-5 report. We have focused our review on the broad issues of assessment structure, justification and clarity set out as review criteria in Section 1. We illustrate our general comments with more detailed comments where appropriate. Further detailed comments by GSL relating to the treatment of colloids in the SFL 3-5 PA can be found in Wickham *et al*. (2000).

Section 1 Introduction

This section sets out the background, purpose and outline of the SFL 3-5 report. It summarises the role of the SFL 3-5 PA and the links between the reported assessment and that undertaken for three hypothetical sites for the disposal of spent fuel (SR 97). The intended role of the SFL 3-5 report in any regulatory decision-making process is not explained, although the purpose of the report is stated to be a preliminary safety assessment. Safety is not an absolute concept, and an assessment of safety must be made against some criteria or target. SR 97 acknowledges the recent introduction of a risk criterion in Swedish regulations on radioactive waste disposal (SSI, 1999), and takes some steps towards undertaking a risk analysis to demonstrate compliance with this criterion. The SFL 3-5 assessment, however, has only a passing reference to the applicable regulations (in Section 8.6.2), and there is no indication that an assessment of overall uncertainties has been undertaken as required by a risk analysis.

Section 2 Inventory

There are extensive discussions and tabulations of the waste forms, radionuclides and radiotoxicity of the inventory that form the basis of the SFL 3-5 assessment (Sections 2.2, 2.3 and 2.4). Section 2.5, however, reveals that there are considerable uncertainties in the inventory. These stem from uncertainties in the components and materials to be consigned to the SFL 3-5 repository and from uncertainties in the radionuclide content of these components. Some uncertainties are acknowledged to be ±70%, but there is no structured assessment of the uncertainties that would indicate the overall uncertainty in the disposed inventory. Further, many of the expert judgements made to establish parameter values for the PA are only discussed at a generic level, e.g., use of correlation factors where data are lacking, use of data for a single reactor to estimate waste volumes from all similar reactors, and estimation of neutron-induced activity. It is not clear if or where these judgements are analysed in detail to estimate the resulting uncertainty. Without this information, it is difficult to assess the effect of the assumptions made on the overall assessment results.

The lack of quantified justification of the treatment of uncertainty is exemplified by the needless use of two sets of radionuclide half-lives for different parts of the assessment (p. 2-14). The reason for using two sets is not provided; instead a statement is made that the effect of the differences is negligible in comparison to other uncertainties. The

statement seems to be based on expert judgement only, and is not supported by any quantitative evaluation.

Section 3 Repository Design

Section 3 presents a design for the SFL 3-5 repository that is quite detailed in terms of the development stage of the concept. SKB acknowledges this, and notes that the reason is to allow more detailed modelling of the near-field environment. The conceptual models of the near-field environment (Section 8) are, however, simplified representations that do not appear to account for potentially significant aspects of the detailed design. For example, there will be voids at the top of the gravel backfill that could have an effect on both fluid flow (groundwater and gases from waste degradation) and the mechanical stability and hydrogeological properties of the host rock.

A further reason for developing a detailed design is to assess the amount of constructional materials and backfill that will be present in the repository. Several design changes from the preceding 1993 design (PLAN 93; SKB, 1993) are presented (p. 3-1), but these are neither fully explained nor justified in Section 3. Some of the changes are discussed in Section 10 and in supporting references (e.g., Appendix D of Karlsson *et al.*, 1999; Section 11 of Pettersson *et al.*, 1999), but the reader is not directed to this supporting material. Two of the key changes with respect to the behaviour of the near-field are that the rock chambers will be backfilled with crushed rock, rather than a mixture of crushed rock and bentonite, and that the waste packages in SFL 3 and SFL 5 will be grouted with porous concrete. As a reference for the safety assessment, SKB assumes that Standard Portland Cement will be used throughout the repository. The reasons for this choice and the variation or uncertainty that might be caused by using other types of cement are mentioned (p. 3-10), but not evaluated in any detail.

The effects of the repository operational period on the engineered barriers and the host rock are reviewed and, subsequently, dismissed in Section 3.5. The main supporting work for the review is presented in Karlsson *et al.* (1999), but this report is not referenced. The issues associated with closure and resaturation are discussed qualitatively, but there is little or no quantitative evaluation, for example, of the implications and time it will take for the repository to resaturate (see also Section 6.4.1) and return to its steady-state redox conditions (see also Section 6.6), and of the implications of the initially very high pH (13.5) environment in the cement-filled parts of the repository (see also Section 6.6). In any event, all of these issues are circumvented by simplifying assumptions in the assessment calculations.

Sections 4 and 5 Site Location and Biosphere Description

The SFL 3-5 assessment assumes that the L/ILW repository is located at the same site as the repository for spent fuel. In order to avoid thermal and chemical interactions between the two repositories, they would, in practice, be some distance apart, even if they shared common access shafts and surface facilities. This separation is shown on

the maps of the "hypothetical" sites in Section 4, and discharge points for groundwater passing through the SFL 3-5 repository are shown on representations of the biosphere at each of the three sites. The separation is set at 1 km, but this is apparently arbitrary and based on expert judgement, and is not justified on a site-specific basis by consideration of chemical and thermal transport.

This approach is appropriate, as it allows hydrogeological models developed as part of SR 97 to be used. The "realism" imposed by this approach may, however, detract to some extent from the assessment as it leads to differences between the sites that may have a strong influence on the calculated results and obscure the effects of other assumptions. This most obviously applies in the treatment of the surface environment. Different biospheres are used in the calculations of dose at the three sites, and these have at least as much influence on the calculated doses as differences in water chemistry and hydrogeological setting. It would be more appropriate to use a reference biosphere to explore differences between the three sites, and to investigate the effects of different biospheres on doses from a given release at a site.

Section 6 Reference Scenario

This section presents a Reference Scenario for the SFL 3-5 PA. This scenario is intended to include the features, events and processes (FEPs) that would occur during the "expected" evolution of the near-field but with the premise of uniform conditions in the far-field. It is not, therefore, a scenario that represents the expected evolution of the disposal system as a whole, because changes in the far-field are not included. This is an appropriate approach for developing an understanding of near-field behaviour, but it is not an appropriate basis for regulatory decision-making because it does not examine all sources of uncertainty. As noted above, the use of different biospheres seems inappropriate in an assessment that assumes uniform far-field conditions and is clearly not intended to explore the whole range of uncertainties.

Section 6 includes brief discussions of a number of processes that are expected to take place within the near-field. Few if any of these processes are, however, carried through to the conceptual model of repository evolution. The reasons for omitting processes from the near-field model are not, in general, made explicit. There are references to other documents in support of statements about the rates of some of the omitted processes, but no references to supporting calculations to show that they can be omitted on the basis of low consequence to the overall performance of the SFL 3-5 disposal system. Similarly, there are no references in the main report to support the use of parameter values that are stated by SKB to be conservative estimates.

There is no formal documentation in the report of a FEP list to demonstrate comprehensiveness, and the THMC (Thermal, Hydrological, Mechanical, Chemical) diagram, which supposedly show processes, events, and their interactions, is not actually presented. The reference scenario used in an earlier assessment of the SFL 3-5 concept (Wiborgh, 1995) was developed using the Process Influence Diagram (PID) methodology. SKB states that the material supporting the development of this scenario has been re-examined and that the results are "summarized" in Section 6. However, the lack of supporting references and formalisation makes the ownership and review/sign-

off of the expert decisions involved in scenario development for the SFL 3-5 PA difficult to trace.

The discussion of the thermal evolution in Section 6.3 is brief, and is supported by reference to Skagius *et al.* (1999b). In the main SFL 3-5 report, SKB states that "… after closure, radioactive decay in the waste is the only process that generates heat", and radioactive decay is the only heat-generating process that is considered in Skagius *et al.* (1999b, Section 5). This presumably relies on the assumption that any contribution to heat generation from exothermic reactions in the concrete backfill and grout is negligible. This assumption should be justified with discussion of the potential for, and impacts of, higher temperatures due to concrete hydration both before and after closure.

Sections 6.6 and 6.7 discuss hydrochemical conditions and barrier properties and how these may change over time. However, the complexity of these discussions is not reflected by the simplicity of the assessment calculations in Section 8. For example, the near-field porewaters are assumed to have either a pH of 12.5 in cement-filled areas or that of the *in situ* groundwater elsewhere. However, higher pH values of 13.5 can be expected at early times in cement-filled areas, the pH will drop in these areas beyond around 100 000 years, and the *in situ* groundwater composition is also likely to change over a timescale of thousands to tens of thousands of years. No evaluation is presented of the effects of uncertainty in hydrochemical conditions and barrier properties or near-field performance. SKB states (in Section 9) that the changing groundwater composition is covered by the range of results from the sites with a fresh and a saline groundwater. This is a rather simplistic view and does not consider holistically the effect of repeated changes in groundwater conditions coupled with other climatic and hydrogeological changes (see review of Section 9 below).

Mineralogical and porosity changes related to the use of large amounts of cement in the disposal concept, and the consequences of a plume of alkaline groundwater are dismissed rather summarily in Section 6, and a constant high porosity (30%) is assumed for the gravel fill (the main hydraulic pathway) in Section 8. There is no quantitative evaluation of the significance of porosity changes and of the possible creation of flow heterogeneity and preferential pathways.

As a further example of the issue of inadequate documentation of FEPs and the basis for their omission, the following comments on how colloids have been treated have been summarised from GSL's recent evaluation of colloid treatment in assessments (Wickham *et al*., 2000):

- SKB assumes that only low concentrations of colloids will be produced from the cementitious materials in the SFL 3-5 repository, based on studies of the Maqarin natural analogue site, where only low colloid concentrations have been observed in high-pH groundwaters that are similar to those expected in the SFL 3-5 repository. There are, however, a number of colloid types and colloid formation processes that should be discussed before a general conclusion is drawn on the role of colloids. Colloid types include actinide intrinsic colloids (e.g., polymeric plutonium), inorganic colloids (e.g., mineral fragments), organic colloids (e.g., humic and fulvic acids), and microbes (e.g., bacteria), and colloids may be formed by several processes, including waste degradation and chemical precipitation at steep chemical

gradients within the repository system (e.g., at the boundary between the high-pH near-field and the near-neutral far-field).

- SKB argues that the transport of colloids from the waste may be limited by anion exclusion. This argument is supported by reference to studies of colloids in a system with a bentonite backfill, rather than with crushed rock as is proposed for the SFL 3-5 repository. Also, although anion exclusion may restrict the transport of certain anionic species by excluding them from small pore spaces, these same species may be concentrated at the centre of larger pore spaces and flow paths such as fractures. As flow velocities are relatively greater in the centre of such preferential pathways, the effect of anion exclusion may be to enhance the transport of anionic species including colloids.

Section 7 Hydrology Calculations

Section 7 presents hydrological calculations for the near-field (Sections 7.2 and 7.3) and far-field (Section 7.4) at each of the three "hypothetical" sites. Section 7.3 is one of the few examples where the effect of uncertainty is discussed, with an evaluation of the effects of changes in repository design and barrier properties on flow rates in the near-field. However, it is unclear how the results of these evaluations have influenced the assumptions made in the assessment calculations. For example, despite there being site-specific data available concerning hydraulic conditions at all three sites, flow through SFL 4 is treated by applying results for Beberg to all three sites. It would appear that uncertainties or unrealistic assumptions have been introduced, and it is not clear why.

The discussion of the far-field in this section presents results from detailed hydrological models for each of the sites, including particle tracking calculations to determine discharge areas. However, the results of these detailed calculations are not used in the remainder of the assessment. Instead, simplified assumptions about travel times from the repository to the surface have been made (with about two orders of magnitude between the fastest and slowest times). This approach could be appropriate for calculations intended to develop an initial understanding of near-field behaviour. A more integrated approach that accounts for uncertainties in each part of the disposal system would, however, be required to support regulatory decision-making.

Section 8 Radionuclide Transport

This section presents the results of radionuclide transport calculations for the near-field and far-field and calculations of dose. Releases of chemotoxic pollutants and gas-phase radionuclides are also briefly summarised.

Radionuclide transport

Flow rates through the far-field and overall flow through the repository are derived from hydrological modelling. Compartment models of the near-field, in which different components (concrete, gravel backfill, etc.) are assigned different permeabilities, are used to determine rates of advection and diffusion within the near-field. Radionuclides

released from the near-field are transported within the far-field by advection, with retardation occurring through sorption on fracture surfaces and diffusion into the rock matrix.

There is a clear statement in Section 8 of the assumptions (premises) used to define the calculational cases. However, there is little, if any, discussion of the basis for these assumptions or of the impact of these on the calculated results. References are given for selected parameter values, but there is no indication of why a particular set of values has been used (e.g., reasonable, pessimistic), nor is there any discussion of parameter uncertainty.

The assumptions that underlie the calculations of dose are less clearly presented. Doses are determined on the basis of mean dose conversion factors for each ecosystem. There is an outline in Section 5 of the assumptions underlying these factors in terms of the transport pathways involved (ingestion, inhalation, surface exposure) and the habits assumed (e.g., fishing, agricultural practices, food consumption patterns). There is an indication of variability of some biosphere parameters in Section 5, but this has not been translated into parameter uncertainty for the dose conversion factors.

The discussion of the dose results acknowledges the applicable regulations, but elects to convert the risk criterion (individual risk to representative member of the most exposed group $< 10^{-6}$ per year) to a dose target (annual dose of 14 ìSv) with the assumption that the probability of exposure is one. There is no discussion of this approach, which has presumably been adopted on the basis that satisfying this dose target would automatically satisfy the risk criterion. All of the dose calculations presented do satisfy this dose target, although some calculated doses are within 50% of the target (note that in Figure 8-10 the target or comparison level has been mis-labelled as the background level). A proper accounting for uncertainties would probably lead to some calculated doses exceeding the dose target. In these circumstances, it would be appropriate for SKB to use a risk-based approach for demonstrating compliance with the risk criterion.

Results of dose calculations are only presented for one ecosystem for each of the three sites. For sites where potential discharges to two different ecosystems are identified, doses arising within the alternative ecosystem are mentioned in terms of dominant radionuclides, but combined dose results have not been presented. As noted above, it would be easier to interpret the influence of different parts of the disposal system if the assessment had used the same reference biosphere for each site. However, since different biospheres and a range of ecosystems have been used, an understanding of the influence of various aspects of the system would be helped if all of the available results were presented.

SKB acknowledges that there are uncertainties in ecosystem evolution. However, despite noting that three glacial periods are expected within the next 100 000 years, the only treatment of uncertainty that has been made is to shade the region representing times *beyond* 100 000 years on the dose-time plots. A more considered approach to the treatment of uncertainty is required if the results are to be used for regulatory decision-making.

Chemotoxic Pollutants

Transport of chemotoxic pollutants from the repository has been calculated in the same manner as transport of radionuclides, although the results of these calculations are not presented. Instead, concentrations have been derived by assuming that the entire inventory of chemotoxic pollutants is transported to the ecosystem. Concentrations are derived by dividing the quantity of material by the volume of the ecosystem. SKB regards this as a conservative assumption, although there is no justification provided for assuming a uniform distribution throughout the ecosystem. It would seem more reasonable to assume that accumulation would be concentrated in smaller regions. The concentrations determined by SKB are stated to be orders of magnitude below comparison levels. These comparison levels are based on mean concentrations measured in different areas. There is no comparison with any regulatory constraints, nor are there any statements regarding the risks posed by either the calculated or the comparison levels.

Gaseous Releases

Consideration of radioactive gas release is restricted to ^{14}C from degradation of organic waste forming a component of methane released from the repository. Comparing the estimated inventory ($<10^5$ Bq) with the corresponding ^{14}C inventory in a spent fuel repository (SR 95; SKB, 1995), and making the same conservative assumption about pulse release, yields a calculated collective dose of 0.04 ìmanSv. Annual individual doses will be still lower. This appears to be a reasonable approach, although additional detail regarding the calculational approach and the assumptions made would be required for a final safety case.

Section 9 Other Scenarios

This section discusses alternative scenarios to the reference case for the evolution of the SFL 3-5 repository. There is discussion of the potential effects of climate change and earthquakes, and of unintentional operational activities. Additional calculations have only been performed, however, for the human intrusion scenario.

Climate Change

The discussion of climate change assumes that the principal effect, in terms of repository performance, will be the periodic growth and retreat of continental-scale ice sheets. The report identifies three domains within the cycle and discusses the effects of these domains on groundwater flow and salinity. The results in terms of radionuclide transport are assumed to be directly related to these changes, and reference is made to results presented in Section 8. The Reference Case results are, however, insufficient to account for all of the changes arising from climate change. For example, there are no results for flow rates greater than those assumed at Aberg, and there is only a direct comparison of the effects of saline and non-saline waters at Beberg. There is also no consideration given to other changes (e.g., length of transport pathways, changes in ecosystem characteristics) arising from climate change.

An assessment to be used for regulatory decision-making will require a clear identification of the FEPs that have an influence on radionuclide transport and dose rates, and documented justification for excluding FEPs from assessment calculations on the basis of low consequence or low probability of occurrence. The material presented in Section 9 for climate change is inadequate on this basis, as it neither incorporates climate change into the analysis of dose rates, nor presents a sufficiently clear argument for excluding climate change from assessment calculations.

Earthquakes

Section 9 also discusses the potential effects of earthquakes on the performance of the SFL 3-5 repository. There are no calculations reported to assess the effects on disposal system performance of possible displacements, and it is therefore unclear as to whether the repository design measures outlined by SKB for reducing these effects are indeed required.

Future Human Actions

The Swedish Radiation Protection Institute (SSI) highlight in their regulation [SSI FS 1998:1] that an assessment of the effects of human activities is required separate from the assessment of the natural evolution of the repository. SKB's decision to consider future human actions as a separate scenario therefore appears appropriate. However, the guidance that accompanies SSI's regulation (SSI, 1999) makes it clear that SSI expects an assessment of the ability of the repository to contain wastes following an intrusion. The future human actions that SKB has considered in Section 9.4 are not intrusive events, and the results presented do not illustrate the long-term behaviour of the repository.

The report presents the results of a review of possible future human actions undertaken for SR 97. These actions are classified according to whether they would have a thermal, hydrological, mechanical or chemical impact on the repository, and include activities such as the building of a heat store or hydroelectric scheme. From this set of human actions, SKB has selected wells drilled in the vicinity of the repository as the activity that defines the Future Human Actions Scenario. However, the assumptions made about these wells are such that they do not have a hydrological or other impact on the repository. The only difference, therefore, between the Future Human Actions Scenario and the Reference Scenario is that different dose conversion factors have been used. This means that the relative contributions of different radionuclides differ between these two scenarios, but there are no changes in the times of peak doses from different radionuclides.

As with the dose conversion factors used in the Reference Case, there is insufficient discussion to understand the assumptions that have been made in deciding how wells are used. The dose conversion factors are described as eco-system dependent, but there is only a limited description of the processes that are assumed to affect radionuclides released via wells. As is the case for the Reference Scenario, comparison of the results between sites for the Future Human Actions Scenario (e.g., Figures 9-9 to 9-11) would be easier if a consistent set of biosphere assumptions was used.

In plots of dose against time for releases from wells, SKB has shaded the region up to 100 years on the basis that institutional controls and societal memory of the repository site would prevent use of wells in the vicinity of the repository during this period. This is a very simplistic approach, and a more detailed consideration should be given to the fate of radionuclides that were not released to the biosphere during a period of institutional controls. For example, the accumulation of radionuclides within an aquifer while controls were in place could lead to higher doses once knowledge of the site was lost and controls became ineffective.

Releases of chemotoxic pollutants to a well are calculated, but are presented only as concentrations in well water. The principal assumption behind this calculation is that the annual release of each pollutant is diluted within the annual capacity of a well. Within the context of the calculation (no bypassing of the near-field), this appears to be a worst case assumption. In this case, regulatory limits for these pollutants are also given for comparison (cf. releases in the Reference Scenario). These show that the calculated releases are several orders of magnitude below the regulatory target.

Design and Operation

The final scenario considered in Section 9 is termed Design and Operation. The only additional FEP considered in this scenario is the presence of stray materials within the repository. SKB has made estimates of the amount of stray organic material and metals/metal oxides that may be left behind in the SFL 3-5 repository. These amounts are likely to be small in comparison to the amounts of organic materials and metals/metal oxides in the overall SFL 3-5 inventory, but will contribute organic material to SFL 4 and SFL 5 where there is normally none in the inventory. SKB has calculated the effects of the organic inventory in SFL 3 on radionuclide transport, and has shown that there are no significant effects during the first million years. The small amounts of stray organic material in SFL 4 and SFL 5 are therefore considered not to be significant. Similarly the effects of stray metals/metal oxides are not considered significant in comparison to the overall effects of metals/metal oxides in the inventory. These comparisons are an appropriate basis for eliminating stray materials from the scenario.

Section 10 Discussion and Conclusions

This final section summarises the conclusions of the preliminary assessment, discusses differences between this assessment and earlier studies of the SFL 3-5 concept, and makes recommendations for future work.

In analysing the results of the assessment, the mixture of realism (i.e., use of site-specific data), conservative assumptions, and simplifying assumptions for the sake of a preliminary assessment creates confusion. The calculated doses cannot easily be related to a coherent set of assumptions, although there is material in this section that uses these results as a basis for decision analysis, design evaluation, and the identification of key issues and uncertainties. The discussion of these issues is, however, somewhat cursory, and a much more detailed and precise set of lessons and proposed future actions might be expected from an assessment at the current stage of SKB's programme.

3 Overall Comments

In this Section, we summarise our comments on the SFL 3-5 assessment, and express them in accordance with the review criteria set out in Section 1.

Overall Approach to PA

Recently introduced regulations in Sweden have established an individual risk criterion ($<10^{-6}$ per year) for the long-term performance of repositories for the disposal of radioactive wastes. SKB has not focused its assessment of SFL 3-5 on demonstrating compliance with this regulation. Instead, SKB has calculated individual dose and provided a comparison with an annual individual dose of 14 ìSv (derived from the risk criteria using the ICRP's dose-risk conversion factor of 0.073 per Sv). The justification of this approach is that probabilities do not need to be determined if doses are less than the dose equivalent to the risk criterion. However, there is insufficient information regarding uncertainty provided in the documentation of the SFL 3-5 assessment to determine whether this approach is reasonable.

SKB's parallel assessment of a repository for spent fuel using the KBS-3 concept (SR 97) accounts for uncertainty by specifying a "reasonable" and a "pessimistic" value for uncertain parameters in the assessment calculations. Although there are problems with the way probabilities have been assigned to these values (Wilmot and Crawford, 2000), this approach does indicate where there are significant uncertainties. The SFL 3-5 PA does not include a structured approach to defining uncertainty, although a number of assumptions and parameter values are stated to be conservative. As a preliminary assessment, there is insufficient information to identify key uncertainties or sensitivities, or to determine where further work should be focused.

Approach to Expert Judgement

Any assessment requires the use of expert judgement to determine how the assessment is conducted, what modelling approach to use, what features, events and processes (FEPs) could potentially affect the disposal system, which FEPs should be included in the conceptual models, and which scenarios should be assessed. Judgements are also required in determining how to parameterise the models, and this may extend to formal expert elicitation for particular parameter values. These uses of expert judgement in assessments are discussed more extensively in a recent study for SKI (Wilmot and Galson, 2000).

The key point to be made about the use of judgements is that they must be documented in such a way that not only can the judgements themselves be examined but so too can the basis for them. Only in this way can judgements be properly reviewed and confidence developed in the results of an assessment based on them.

Very similar comments apply to SFL 3-5 as were made in our review of SR 97 (Wilmot and Crawford, 2000) regarding the use of expert judgement. There is no formal documentation of the expert judgements made at the various stages of the development

of the SFL 3-5 assessment, although the use of expert judgement is recognised by SKB. Therefore, the ownership of the judgements (i.e., who made them, how they were made, and why) cannot be determined, and the review and approval process applied to these judgements cannot be assessed. The assessment is at a preliminary stage, and this may preclude the extensive use of expert elicitation as a judgement tool. However, dialogue and peer review could both be applied beneficially to build confidence in the assessment.

Approach to Definition of Scenarios and Comprehensiveness of the PA

The stated purpose of the SFL 3-5 preliminary assessment is to examine the effects on calculated doses of different hydrological and biosphere conditions. In this sense, it would be appropriate for the assessment to be restricted to a limited set of scenarios, but only if such scenarios were clearly defined and allowed different aspects of the disposal system to be examined and sensitivities to be assessed. In the SFL 3-5 PA, SKB defines four scenarios, of which two have been used for performance calculations – a Reference Scenario and a Future Human Actions Scenario. However, neither of these scenarios adequately fulfil the requirements of clarity or usefulness. The principal issues of concern are:

- There is no structured reporting of a set of potentially important FEPs, or of the basis for omitting FEPs from the assessment calculations.

- The site descriptions used to develop a Reference Scenario for each of the three sites examined include differences in far-field conditions and in the biosphere. This prevents a clear understanding of the role of different groundwater flow rates, because of the significant differences in biosphere characteristics. Use of a reference biosphere at each of the three sites, in addition to more detailed biosphere calculations, would provide a better basis for comparison.

- The Reference Scenario is time-independent and excludes any changes in near-field, far-field or biosphere conditions for a period of 10^7 years.

- The Future Human Actions Scenario is based simply on a change in the dose conversion factors for the biosphere, and does not consider intrusion or bypassing of the near-field barriers.

Overall Clarity and Quality of Presentation of the PA

The overall structure of the main SFL 3-5 PA report is appropriate as a top-level document that summarises the assessment context, disposal system characteristics, key assumptions and results. In general, the report is well written and the material presented can be understood. There are places where there are insufficient cross-references within the document, particularly between the descriptions of the disposal system and the description of how it is modelled.

The key concern is that there are often insufficient references to other documents to fully explain and justify what has been done. A preliminary assessment requires this information just as much as a more detailed assessment. A more through and rigid cross-referencing to more detailed information in the supporting documents would allow reviewers to trace arguments and data to whatever level of detail is required, and would build confidence in the assessment process.

4 References

Karlsson, F., Lindgren, K., Skagius, K., Wiborgh, M. and Engkvist, I. 199. Evolution of geochemical conditions in SFL 3-5. SKB Report R-99-15. SKB, Stockholm.

Pettersson, M., Skagius, K. and Moreno, L. 1999. Analysis of radionuclide migration from SFL3-5. SKB Report R-99-14. SKB, Stockholm.

Skagius, K, Lindgren, M. and Pers, K. 1999a. Gas generation in SFL 3-5 and effects on radionuclide release. SKB Report R-99-16. SKB, Stockholm.

Skagius, K, Pettersson, M., Wiborgh, M., Albinsson, Y. and Holgersson, S. 1999b. Compilation of data for analysis of radionuclide migration from SFL 3-5. SKB Report R-99-13. SKB, Stockholm.

SKB (Swedish Nuclear Fuel and Waste Management Company). 1993. Plan 93. Costs for management of the radioactive waste from nuclear power production. SKB Technical Report 93-28. SKB, Stockholm.

SKB (Swedish Nuclear Fuel and Waste Management Company). 1995 Template for safety reports with descriptive example. SKB Technical Report 96-05. SKB, Stockholm.

SKB (Swedish Nuclear Fuel and Waste Management Company). 1999a. Deep repository for long-lived low- and intermediate-level waste. Preliminary safety assessment. SKB Technical Report TR-99-28. SKB, Stockholm.

SKB (Swedish Nuclear Fuel and Waste Management Company). 1999b. SR 97 – Post-closure safety. Main Report. SKB Technical Report TR-99-06. SKB, Stockholm.

SSI (Swedish Radiation Protection Institute). 1999. Health, Environment and Nuclear Waste: SSI Regulations and Comment. SSI Report 99:02. SSI, Stockholm.

Wickham, S.M., Bennett, D.G. and Higgo, J. 2000. Evaluation of Colloid Transport Issues and Recommendations for SKI Performance Assessments. SKI Report (in press).

Wilmot, R.D. and Crawford, M.B. 2000. A Review of Expert Judgement and Treatment of Probability in SR 97. SKI Report (this volume).

Wilmot, R.D. and Galson, D.A. 2000. Expert Judgement in Performance Assessment. SKI Report 00:4. SKI, Stockholm.

The autors

Dr. Mark B Crawford

Dr. Mark B. Crawford is a Senior Consultant at Galson Sciences Ltd. He has degrees in Geology and Geochemistry from Oxford University (BA) and Leicester University (PhD), and a Diploma in Environmental Impact Assessment. Over the last nine years he has been involved in consultancy and research work in the area of radioactive waste disposal for clients in Finland, France, the UK and the US. This work has included the development of geochemical models for organic complexation in natural systems, validation of sorption modelling within a European Community research initiative, and interpretation of hydrochemical data obtained as part of Nirex's site characterisation programme. He has performed reviews of geochemical techniques in relation to palaeo-hydrogeological studies and of the effects of alkaline plume migration from cementitious waste repositories. He made substantial contributions to the development and review of technical input for the Waste Isolation Pilot Plant (WIPP) Compliance Certification Application, and subsequently in responding to stakeholder comments. He has undertaken review and systems analysis of the WIPP near-field modelling, and helped in development of compliance monitoring strategies. He was involved in a review of scenario development methodologies on behalf of ANDRA in France, and was the lead author for a report describing the normal evolution of a spent fuel repository for the TILA-99 performance assessment study in Finland. He is currently managing a performance assessment for low-level waste disposal in the UK.

Dr. Roger Wilmot

Dr. Roger D. Wilmot is a Senior Consultant at Galson Sciences Ltd. He has degrees in Earth Sciences from Cambridge University (BA) and Imperial College, London (PhD). He is a geologist with over 20 years experience in providing a broad range of research, consultancy and management services to a range of clients. This involvement has included a review of validation in the context of radioactive waste disposal, and the development of guidance concerning the treatment of validation in safety cases. On behalf of Her Majesty's Inspectorate of Pollution and the Environment Agency, he has organised international seminars on "Validation," "Risk Perception and Communication," "Management of Safety Assessments" and "Use of the Expectation Value of Risk." He has recently completed a project on the use of the expectation value of risk, and contributed to a technical and policy review of the HMIP radioactive waste research programme. He has contributed to the development and use of computer codes for incorporating long-term environmental change into safety assessments. Recent work outside the UK has included descriptions of climatic and geomorphological evolution in Finland for POSIVA, a leading role in describing elements of a regulatory strategy for consideration of future human actions in assessments for SKI, and involvement in performance assessment and near-field systems analysis for the WIPP site in the US. He is currently managing an options appraisal for low-level waste management in the UK. Finally, he has experience of several QA programmes, and is the Company's Quality Assurance Manager.