SKI Report 02:53

Research

SFR 1 Vault Database

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SKI perspective

Background

As part of the license for SFR 1 a renewed safety assessment should be carried out at least every ten years for the continued operation of the SFR 1 repository. SKB has at mid-year 2001 finalised their renewed safety assessment (project SAFE) which evaluates the performance of the SFR 1 repository system.

As part of SKI's own capability to perform radionuclide transport calculations a need to develop a database for the near-field of SFR 1 repository was identified.

Purpose of the project

The purpose of this project is to make a compilation of physical and chemical data for the engineered barriers plus near-field rock of the SFR 1 repository.

Results

The parameters in the SFR 1 vault database has successfully been used in SKI's own radionuclide transport calculations and in the review of SKB's safety assessment for SFR 1.

Effect on SKI's work

This project has given SKI not only an updated parameter database for SFR 1 but also partly an useful database for the low and intermediate level waste repository SFL 3-5.

Project information

Responsible at SKI has been Bo Strömberg.

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Relevant SKI report:
Savage, D., Stenhouse, M., Benbow, S., Evolution of Near-Field Physico-Chemical Characteristics of the SFR Repository, SKI Report 00:49, Swedish Nuclear Power Inspectorate, Stockholm, Sweden, 2000.

Chapman, N. A., Maul, P. R., Robinson, P. C., Savage D., SKB's Project SAFE for the SFR 1 Repository - A Review by Consultants to SKI -, SKI Report 02:61, Swedish Nuclear Power Inspectorate, Stockholm, Sweden, 2002.

Maul P. R., Robinson P. C., Exploration of Important Issues for the Safety of SFR 1 using Performance Assessment Calculations, SKI Report 02:62, Swedish Nuclear Power Inspectorate, Stockholm, Sweden, 2002.

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Research

SFR 1 Vault Database

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Summary

SKB is carrying out a safety assessment of the operational SFR 1 repository under the auspices of the 'SAFE' (Safety Assessment of Final Repository for Radioactive Operational Waste) project (SKB, 1998a; SKB, 1998b). SKI in turn, is carrying out its own review of SFR 1.

The work presented here is a compilation of physical and chemical data for the SFR 1 repository which will be used in radionuclide transport and assessment calculations by SKI. This compilation has focused on the repository itself (engineered barriers plus near-field rock).

Data have been compiled for the following:

- Physical properties (porosity, hydraulic conductivity, bulk density, effective diffusivity);
- Sorption of radionuclides (on concrete, sand, bentonite, sand-bentonite, and rock);
- Radionuclide solubility.

In addition, issues affecting gas generation at SFR 1 have been reviewed and placed in context with research conducted for the SFL 3-5 repository.

Sammanfattning

SKB har utfört en säkerhetsanalys på slutförvaret för radioaktivt driftavfall, SFR 1, under ledning av projektet "SAFE" (Safety Assessment of Final Repository for Radioactive Operational Waste) (SKB, 1998a; SKB, 1998b). SKI i sin tur utför sin egen granskning av SFR 1.

I denna rapport presenteras en sammanställning av fysikaliska och kemiska data för SFR 1-förvaret vilka kommer att användas i SKI:s egna radionuklidtransport och analys beräkningar. Denna sammanställningen har sitt fokus på själva förvaret (tekniska barriärer och berget närmast förvaret).

Data har sammanställts för följande områden:

- Fysikaliska egenskaper (porositet, hydraulisk konduktivitet, bulkdensitet, effektiv diffusivitet).
- Sorption av radionuklider (på betong, sand, bentonit och sand-bentonit blandning och berg).
- Löslighet för radionuklider.

Dessutom har frågor som påverkar bildandet av gas i SFR 1 granskats och satt i sitt sammanhang med den forskning som utförts för SFL 3-5-förvaret.

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1 Introduction

SKB is carrying out a safety assessment of the operational SFR 1 repository under the auspices of the ‘SAFE’ (Safety Assessment of Final Repository for Radioactive Operational Waste) project (SKB, 1998a; SKB, 1998b). SKI in turn, is carrying out its own review of SFR 1.

The work presented here is a compilation of physical and chemical data for the SFR 1 repository which will be used in radionuclide transport and assessment calculations by SKI. This compilation has focused on the repository itself (engineered barriers plus near-field rock).

Consideration has been given to the changes in physical and chemical properties of barriers with time due either to physicochemical degradation of the engineered barrier system resulting from groundwater flow and chemical reaction, and/or geological evolution of the site resulting in uplift/subsidence and consequent emergence or submergence beneath the Baltic Sea. These latter processes are thought to induce changes in groundwater chemistry. Consequently, evolution of the SFR 1 site has been divided into the time-dependent stages, according to processes described elsewhere (Savage et al., 2000).

Stage I, which is representative of 'fresh' cementitious barriers and cement pore fluid conditions of pH 12.5-13. Portlandite [$CaOH)_2$] and CSH gel are present in the system.
Stage II, which is representative of partially degraded cementitious barriers, corresponding to cement pore fluid conditions controlled by the solubility of portlandite (pH 12.5). Partial removal of portlandite is assumed to have occurred.
Stage III, which is representative of partially degraded cementitious barriers, corresponding to cement pore fluid conditions controlled by CSH gel ($pH < 12$). Portlandite has been removed. Partial removal of CSH gel is assumed to have occurred.

Since different parts of SFR 1 have different amounts of concrete, this time-evolution of physicochemical conditions will not occur at the same rate throughout SFR 1. Savage et al. (Savage et al., 2000) have pointed out that although the Silo, BMA and BTF vaults may have pore fluids with $pH > 10$ for upwards of 10^6 a, the BLA vault may be exposed to ambient groundwater conditions almost immediately after closure.

Superimposed upon each of the three stages identified above are the effects of subsidence and uplift and concomitant effects upon groundwater composition. Consequently, each of the stages could be accompanied by the presence of 'fresh' and 'saline' groundwater. These different groundwater types could affect sorption, solubility and diffusivity of radionuclides.

For the most part, Swedish data for the various barrier properties have been selected for inclusion in the database, because of their relevance to the specific materials concerned. Where possible, the selection of data for inclusion in the database has taken into account relevant data from safety assessments conducted elsewhere, e.g. the United Kingdom, Switzerland, USA etc. However, care has been taken that any data thus obtained should be relevant to disposal conditions at SFR 1.

2 Physical properties data

This section of the report considers data availability for porosity, hydraulic conductivity, density, and diffusivity of radionuclides in the engineered barriers and near-field rock of SFR 1. For the most part, these data are obtained from previous work by SKB either specifically for SFR 1, or relevant portions of the planned SFL 3-5 repository for intermediate-level radioactive wastes.

2.1 Porosity

Porosity data for the SFR 1 system are presented in Table 2.1.

2.1.1 Waste matrices

Data for the porosity of waste matrices was taken from SKB data (Allard et al., 1991, as quoted by Höglund and Bengtsson, 1991). It is considered that these data are the most relevant for the different materials within the waste containers at SFR 1. The initial porosity values range from 0.1 to 0.7, depending upon the precise nature of the concrete. Changes to initial porosity values due to partial dissolution of portlandite (Stage II) and CSH gel (Stage III) were also taken from Höglund and Bengtsson (Höglund and Bengtsson, 1991). As concluded by Höglund and Bengtsson (1991), it is assumed that dissolution of portlandite produces negligible changes to porosity. The uncertainty quoted for each porosity value reflects the range of values quoted by Höglund and Bengtsson (1991).

The porosity value considered by Nagra (Nagra, 1994b) for concrete inside waste containers was 0.25. Nagra did not consider explicitly changes in porosity values due to concrete degradation.

2.1.2 Concrete

Data for the porosity of porous and structural concrete were taken from SKB data (Allard et al., 1991, as quoted by Höglund and Bengtsson, 1991), with provisos as described under Section 2.1.1.

Porosity values considered by Nagra (1994b) for structural and porous concrete in the planned Wellenberg repository for intermediate-level waste were 0.05 and 0.35, respectively. Time-dependent variation of porosity was not considered.

UK Nirex Ltd quote a value of 0.5 for the porosity of their 'Nirex Reference Vault Backfill' (NRVB) cement (Francis et al., 1997).

2.1.3 Bentonite, sand-bentonite, sand, backfill

Data for the porosities of bentonite, sand-bentonite, and sand were taken from Allard et al., (1991) [as quoted by Höglund and Bengtsson, 1991], and the porosity value for rock backfill was taken from the analysis of the SFL 3-5 repository by Skagius et al. (1999).

These sources do not quote uncertainties for porosity values, but it is estimated that the values could vary by ± 10 % due to potential variations in materials and emplacement methods. In the absence of any data concerning the interaction of these materials with cement pore fluids, it is assumed that the porosity of these materials does not change with time.

From its review of a number of safety assessments of the disposal of HLW in fractured hard rock, Safety Assessment Management Ltd (SAM, 1996) presented the following porosity values for bentonite: SKB 91 (Sweden) 0.25; TVO 92 (Finland) 0.43; Kristallin-1 (Switzerland) 0.38; PNC H-3 (Japan) 0.33; AECL 94 (Canada) 0.40. The value selected for SFR 1 (0.25) is thus at the lower end of this range.

Note that for some elements, specifically those that exist in solution as anions, a reduced transport porosity is normally provided to account for anion exclusion in compacted bentonite. Thus, for SKB 91 reduced porosities of 0.05 were provided for Cl, Tc (oxidising conditions) and I; for TVO 92, reduced porosities of 0.05 were provided for C, Cl, Se, Tc (oxidising conditions) and I.

2.1.4 Near-field rock

The porosity values for near-field rock fractures and near-field rock matrix were taken from the typical values for Swedish rock used in the analysis of the SFL 3-5 repository (Ohlsson and Neretnieks, 1997, as quoted by Skagius et al., 1999). These range from 0.001 to 0.01 for the rock matrix and from 0.0004 to 0.02 for the rock fractures.

Ohlsson and Neretnieks (1997) suggest that the porosity available for anions should be less than that available for cations, due to so-called 'anion exclusion' processes and propose porosity values a factor of 10 less for radionuclides such as ^{14}C, ^{36}Cl and ^{129}I. These potential porosity differences for anions and cations have not been included in the study described here.

For its safety assessment of the disposal of HLW in fractured hard rock in Switzerland, Nagra (1994b) considered that the porosity of fracture fills was 0.02-0.03, depending upon the mineralogical alteration of the infill. The porosity of the wall-rock was considered to be 0.0025-0.05, depending upon its state of alteration. These values are both somewhat greater than those adopted here, but clearly, Nagra's values relate to site-specific rock material in Switzerland.

2.2 Hydraulic conductivity

Hydraulic conductivity data for the SFR 1 system are presented in Table 2.1.

2.2.1 Waste matrices

No hydraulic conductivity data specific to the materials within the waste containers at SFR 1 could be found. In the absence of these data it is suggested that the hydraulic conductivity data for porous concrete (below) are adopted for safety assessment calculations (0.3 ± 0.2 m y^{-1}).

2.2.2 Concrete

Höglund and Bengtsson (1991) quote a hydraulic conductivity value for unfractured, fresh concrete as $< 3\times10^{-4}$ m y^{-1}, and that for fractured concrete as $> 3\times10^{-1}$ m y^{-1}. 'Porous' and 'structural' concrete types were not distinguished.

Nagra (Nagra, 1994a) considered three different sets of hydraulic conductivity values for concrete according to their degree of understanding for their safety assessment of an intermediate-level waste repository at the Wellenberg site in Switzerland. These different values were termed 'optimistic', 'realistic' and 'pessimistic'. Time-dependent variation of this parameter was not considered as such. For structural concrete, these values ranged from 3×10^{-3} to 3×10^{-4} m y^{-1} ('optimistic') through 3×10^{-3} to 3×10^{-2} m y^{-1} ('realistic'), to 3×10^{-1} m y^{-1} ('pessimistic'). For relatively porous concrete backfill (porosity = 0.35), Nagra suggest a hydraulic conductivity value of 3×10^{-1} m y^{-1} (identical in 'optimistic', 'realistic' and 'pessimistic' cases).

UK Nirex Ltd quote a value of 3×10^{-2} m y^{-1} for the hydraulic conductivity of their 'Nirex Reference Vault Backfill' (NRVB) cement (Francis et al., 1997). NRVB has a relatively high porosity of 0.5.

In view of the sparseness of data specific to SFR 1, it is suggested that hydraulic conductivity data for stages I, II, and III are similar to those suggested by Nagra (1994a), namely, for structural concrete $3\times10^{-3} \pm 2\times10^{-3}$, $3\times10^{-2} \pm 2\times10^{-2}$, and $3\times10^{-1} \pm 2\times10^{-1}$ m y^{-1}, respectively, and for porous concrete, a value of $3\times10^{-1} \pm 2\times10^{-1}$ m y^{-1} throughout stages I, II and III.

2.2.3 Bentonite, sand-bentonite, sand, backfill

From its review of safety assessments of the disposal of HLW in fractured hard rock in Switzerland, SAM (1996) report hydraulic conductivity values for bentonite measured by high-pressure techniques as $< 3\times10^{-6}$ m y^{-1} (Sweden, Switzerland, Finland, Japan) or $< 3\times10^{-4}$ m y^{-1} (Canada).

Hydraulic conductivity measurements carried out using ultracentrifuge methods (e.g. Conca et al., 1993) report values below detection limits (3×10^{-6} m y^{-1}), emphasising that once water-saturation is achieved, bentonite is water impermeable and that solute transport occurs by diffusion only.

The value quoted by Conca et al. (1993) is proposed for both bentonite and sand-bentonite mixes at SFR 1. It is assumed that this value is time-invariant in the absence of any SFR 1-specific data concerning the potential interaction of cement pore fluids with bentonite. It is considered that these interactions could increase or decrease hydraulic conductivity.

2.2.4 Near-field rock

Höglund and Bengtsson (1991) quote a value for the hydraulic conductivity of the rock around SFR 1 as 0.5 m y^{-1}. Skagius et al. (1999) quote hydraulic conductivity values for Swedish rock in the range 3×10^{-3} to 2×10^{2} m y^{-1}. It is assumed that hydraulic conductivities for the rock matrix are at the lower end of this range, whereas those for fractures are at the higher end of the range. Values of 0.3 (range 0.003 to 3) and 10 (range 1 to 100) m y^{-1} were therefore selected for the rock matrix and near-field fractures, respectively, at SFR 1.

Table 2.1 Porosity and hydraulic conductivity data during 'Stages I, II, and III' of repository evolution.

	Porosity			**Hydraulic conductivity (m y^{-1})**		
Evolution Stage	I	II	III	I	II	III
Silo: walls, bottom, lid	0.125 [a] ±0.025	0.125 [a] ±0.025	0.25 [a] ±0.1	-	-	-
Silo: porous concrete	0.5 [a] ±0.1	0.5 [a] ±0.1	0.6 [a] ±0.1	-	-	-
Silo: compartment walls	0.125 [a] ±0.025	0.125 [a] ±0.025	0.25 [a] ±0.1	-	-	-
Silo: moulds	0.125 [a] ±0.025	0.125 [a] ±0.025	0.25 [a] ±0.1	-	-	-
Silo: conditioning cement	0.2 [a] ±0.02	0.2 [a] ±0.02	0.6 [a] ±0.1	-	-	-
BMA: construction concrete	0.125 [a] ±0.025	0.125 [a] ±0.025	0.25 [a] ±0.1	-	-	-
BMA: moulds	0.125 [a] ±0.025	0.125 [a] ±0.025	0.25 [a] ±0.1	-	-	-
BTF: construction concrete	0.125 [a] ±0.025	0.125 [a] ±0.025	0.25 [a] ±0.1	-	-	-
BTF: moulds	0.125 [a] ±0.025	0.125 [a] ±0.025	0.25 [a] ±0.1	-	-	-
BTF: porous concrete	0.5 [a] ±0.1	0.5 [a] ±0.1	0.6 [a] ±0.1	-	-	-
Porous concrete	0.5 [a] ±0.1	0.5 [a] ±0.1	0.6 [a] ±0.1	3E-1 [d] ±2E-1	3E-1 [d] ±2E-1	3E-1 [d] ±2E-1
Structural concrete	0.125 [a] ±0.1	0.125 [a] ±0.1	0.25 [a] ±0.1	3E-3 [d] ±2E-3	3E-2 [d] ±2E-2	3E-1 [d] ±2E-1
Bentonite	0.25 [a] ±0.1	0.25 [a] ±0.1	0.25 [a] ±0.1	<3E-6 [e]	<3E-6 [e]	<3E-6 [e]
Sand-bentonite	0.6 [a] ±0.1	0.6 [a] ±0.1	0.6 [a] ±0.1	<3E-6 [d]	<3E-6 [d]	<3E-6 [d]
Sand	0.3 [a] ±0.1	0.3 [a] ±0.1	0.3 [a] ±0.1	3E3 [f] (3E1 - 3E5)	3E3 [f] (3E1 - 3E5)	3E3 [f] (3E1 - 3E5)
Backfill	0.3 [b] ±0.1	0.3 [b] ±0.1	0.3 [b] ±0.1	3E3 [f] (3E1 - 3E5)	3E3 [f] (3E1 - 3E5)	3E3 [f] (3E1 - 3E5)
Near-field rock fractures	0.001 [b] (0.0004 - 0.02)	0.001 [b] (0.0004 - 0.02)	0.001 [b] (0.0004 - 0.02)	1E1 [b] (1E0 - 1E2)	1E1 [b] (1E0 - 1E2)	1E1 [b] (1E0 - 1E2)
Near-field rock matrix	0.005 [c] (0.001-0.01)	0.005 [c] (0.001-0.01)	0.005 [c] (0.001-0.01)	3E-1 [c] (3E-3 - 3E0)	3E-1 [c] (3E-3 - 3E0)	3E-1 [c] (3E-3 - 3E0)

[a] Allard et al. (1991), as quoted by Höglund and Bengtsson (1991). [b] Skagius et al. (1999). [c] Ohlsson and Neretnieks, 1997, as quoted by Skagius et al. (1999). [d] See text. [e] Conca et al. (1993). [f] Freeze and Cherry, 1979, as quoted by Skagius et al. (1999).

2.3 Bulk density

Bulk density values of materials in the SFR 1 repository are presented in Table 2.2.

Densities are quoted taking into account porosity values from Table 2.1. It is assumed that porosity is filled with air.

2.3.1 Waste matrices

The densities of concrete filling the various waste structures in SFR 1 were calculated using the porosity values from Table 2.1 (from Höglund and Bengtsson, 1991) and a density of concrete of 2400 kg m^{-3} (from Skagius et al., 1999). Density values are identical for repository evolution stages I and II, but decrease according to changes in porosity (Table 2.1) for stage III.

The density value considered by Nagra (1994a) for concrete inside waste containers was 1350 kg m^{-3} which is at the lower end of the range of initial values used here (1200-2100 kg m^{-3}).

2.3.2 Concrete

Generic densities for 'porous' and 'structural' concrete included in Table 2.2 are those calculated using porosity data from Table 2.1 (from Höglund and Bengtsson, 1991) and a density of concrete of 2400 kg m^{-3} (from Skagius et al., 1999).

For their safety assessment of an intermediate-level waste repository at the Wellenberg site in Switzerland (Nagra, 1994b) considered density values for various concretes in the repository structure. For cavern linings and container walls, the density was 500 kg m^{-3}, whereas the density of cavern infill and container lids was 1700 kg m^{-3}.

The density of UK Nirex's NRVB (50 % porosity) is 1095 kg m^{-3} (Francis et al., 1997).

2.3.3 Bentonite

For its safety assessment of the disposal of HLW in fractured hard rock in Switzerland, Nagra (1994b) considered that the solid density ('specific density') of bentonite was 2760 kg m^{-3}. This value translates to a bulk density of 1767 kg m^{-3} assuming a porosity of 0.36. This value has been used to calculate the density of bentonite at SFR 1, using the porosity data from Table 2.1.

2.3.4 Near-field rock

The density of granitic rock was assumed to be 2700 kg m^{-3} (Krauskopf and Bird, 1995) with values in Table 2.2 being calculated from the porosity values in Table 2.1.

2.4 Effective diffusivity

Effective diffusivity data are presented in Table 2.2. Data are compatible with the following formula:

$$D_e = \varepsilon D_0 \frac{\delta_d}{\tau^2} \qquad [2.1]$$

where D_e is the effective diffusivity ($m^2\ y^{-1}$), ε is porosity (m^3/m^3), D_0 is the diffusivity in unconfined pore water ($m^2\ y^{-1}$) δ_d is a constrictivity factor describing the number of narrow passages in the pore structure, and τ^2 is a tortuosity factor describing the tortuosity of pores.

It can be seen from equation [2.1] that effective diffusivity is directly proportional to porosity and the 'geometric factor', δ_d/τ^2. Consequently, each effective diffusivity value in Table 2.2 has an associated porosity and geometric factor (apart from those for the near-field rock matrix and near-field rock fractures where geometric factor data are missing).

Effective diffusivity values presented in Table 2.2 were calculated assuming a uniform diffusivity in unconfined water (D_0) of $6\times10^{-2}\ m^2\ y^{-1}$ (Höglund and Bengtsson, 1991).

2.4.1 Waste matrices

Effective diffusivity data for concretes used as waste matrices in Table 2.2 were calculated using the porosity data from Table 2.1, a free pore water diffusion coefficient of $6\times10^{-2}\ m^2\ y^{-1}$, and 'geometric factors' of 0.01, 0.1 and 0.25 for stages I, II and III respectively for 'structural' concrete (in lids, compartment walls etc), and a 'geometric factor' of 0.5 for stages I - III for 'porous' concrete. The values for geometric factors for fresh and degraded concrete are as recommended by Höglund and Bengtsson (1991).

2.4.2 Concrete

As above, effective diffusivity data for porous and structural concretes in Table 2.2 were calculated using the porosity data from Table 2.1, a free pore water diffusion coefficient of $6\times10^{-2}\ m^2\ y^{-1}$, and 'geometric factors' of 0.01, 0.1 and 0.25 for stages I, II and III respectively for 'structural' concrete (in lids, compartment walls etc), and a 'geometric factor' of 0.5 for stages I - III for 'porous' concrete. The values for geometric factors for fresh and degraded concrete are as recommended by Höglund and Bengtsson (1991).

For their safety assessment of an intermediate-level waste repository at the Wellenberg site in Switzerland Nagra (1994a) considered 'pore diffusion constants' for various concretes in the repository structure to be in the range 0.003 to 1.3 $m^2\ y^{-1}$, which are generally greater than those presented in Table 2.2.

UK Nirex Ltd measured effective diffusion coefficients in the range 3×10^{-3} to 2×10^{-2} m^2y^{-1} for their (porous) NRVB concrete backfill. These values are very similar to those presented in Table 2.2.

2.4.3 Bentonite, sand-bentonite, sand, backfill

Data for the effective diffusivity of bentonite and sand-bentonite mixes were taken from the work of Höglund and Bengtsson (1991) which are regarded as the most relevant for materials used in SFR 1. These authors quote 'geometric factors' for bentonite and sand-bentonite as 0.2 and 0.08, respectively. Uncertainties quoted for effective diffusivity values are those associated with porosity estimates.

From its review of safety assessments of the disposal of HLW in fractured hard rock, Safety Assessment Management Ltd. (1996) quote values for the effective diffusivity of bentonite in the range 1×10^{-5} to 9×10^{-3} $m^2\ y^{-1}$. The value selected here for SFR 1 (3×10^{-3} $m^2\ y^{-1}$) is at the upper end of this range and corresponds to the value used in SKB 91 (Brandberg and Skagius, 1991).

Data for the effective diffusivity of sand and rock backfill were taken from the work of Skagius et al. (1999) for the SFL 3-5 repository. A geometric factor of unity was assumed for both materials.

In the absence of any data concerning the interaction of cement pore fluids with these materials (bentonite, sand-bentonite, sand, rock backfill), time-invariant values were chosen.

2.4.4 Near-field rock

Data for the effective diffusivity of the near-field rock matrix were taken from the work of Skagius et al. (1999) for generic Swedish rock. However, these data were re-worked assuming a free pore water diffusion coefficient of 6×10^{-2} $m^2\ y^{-1}$ to achieve consistency with data used for diffusion in the EBS, rather than the value of 3×10^{-2} $m^2\ y^{-1}$ chosen by Skagius et al. (1999). Interestingly, Skagius et al. (1999) chose a different free pore water diffusion coefficient value for the engineered barrier materials (6×10^{-2} $m^2\ y^{-1}$) from that employed for the near-field rock (3×10^{-2} $m^2\ y^{-1}$) for their assessment of the behaviour of the SFL 3-5 repository. A rather large diffusion depth of 2-20 m into the rock matrix was employed by Skagius et al. (1999). A more realistic value for diffusion distances in fractured hard rock would be 5-10 cms (e.g. Nagra, 1994b).

Skagius et al. (1999) also present different effective diffusivity data for different radionuclides as well as different data for 'fresh' and 'saline' groundwater. Some radionuclides were considered to have a ten times greater effective diffusion coefficient in saline groundwater due to 'anion exclusion' (inorganic carbon, Cl, I), whereas others were assumed to have a diffusion coefficient ten times lower (Cs, Sr). Diffusion coefficients for other radionuclides were identical in the two groundwater types. Such differences for different radionuclides and different pore waters are not reproduced here. Instead, note has been taken of the range of data presented by Skagius et al. (1999) and a mean value selected in Table 2.2 (2×10^{-6} $m^2\ y^{-1}$). The range of data identified by Skagius et al. (1999) is here used as a range of uncertainty for safety calculations. Unlike other effective diffusivity data, these values are not linked to specific porosity and geometric factor data.

In the absence of any other data, the effective diffusivity data for the near-field rock matrix were also used for near-field rock fractures.

Table 2.2 Bulk density and effective diffusivity data during 'Stages I, II, and III' of repository evolution.

	Bulk density, kg m^{-3}			**Effective diffusivity, m^2 y^{-1} [Geometric factor', δ_d/τ^2]**		
Evolution Stage	I	II	III	I	II	III
Silo: walls, bottom, lid	2100[a] ±60	2100[a] ±60	1800[a] ±240	8E-5 ±2E-5[b] [0.01]	8E-4 ±2E-4[b] [0.1]	4E-3 ±2E-3[b] [0.25]
Silo: porous concrete	1200[a] ±240	1200[a] ±240	960[a] ±240	2E-2 ±3E-3[b] [0.5]	2E-2 ±3E-3[b] [0.5]	2E-2 ±3E-3[b] [0.5]
Silo: compartment walls	2100[a] ±60	2100[a] ±60	1800[a] ±240	8E-5 ±2E-5[b] [0.01]	8E-4 ±2E-4[b] [0.1]	4E-3 ±2E-3[b] [0.25]
Silo: moulds	2100[a] ±60	2100[a] ±60	1800[a] ±240	8E-5 ±2E-5[b] [0.01]	8E-4 ±2E-4[b] [0.1]	4E-3 ±2E-3[b] [0.25]
Silo: conditioning agent	1920[a] ±50	1920[a] ±50	960[a] ±240	2E-2 ±3E-3[b] [0.5]	2E-2 ±3E-3[b] [0.5]	2E-2 ±3E-3[b] [0.5]
BMA: construction concrete	2100[a] ±60	2100[a] ±60	1800[a] ±240	8E-5 ±2E-5[b] [0.01]	8E-4 ±2E-4[b] [0.1]	4E-3 ±2E-3[b] [0.25]
BMA: moulds	2100[a] ±60	2100[a] ±60	1800[a] ±240	8E-5 ±2E-5[b] [0.01]	8E-4 ±2E-4[b] [0.1]	4E-3 ±2E-3[b] [0.25]
BTF: construction concrete	2100[a] ±60	2100[a] ±60	1800[a] ±240	8E-5 ±2E-5[b] [0.01]	8E-4 ±2E-4[b] [0.1]	4E-3 ±2E-3[b] [0.25]
BTF: moulds	2100[a] ±60	2100[a] ±60	1800[a] ±240	8E-5 ±2E-5[b] [0.01]	8E-4 ±2E-4[b] [0.1]	4E-3 ±2E-3[b] [0.25]
BTF: porous concrete	1200[a] ±240	1200[a] ±240	960[a] ±240	2E-2 ±3E-3[b] [0.5]	2E-2 ±3E-3[b] [0.5]	2E-2 ±3E-3[b] [0.5]
Porous concrete	1200[a] ±240	1200[a] ±240	960[a] ±240	2E-2 ±3E-3[b] [0.5]	2E-2 ±3E-3[b] [0.5]	2E-2 ±3E-3[b] [0.5]
Structural concrete	2100[a] ±60	2100[a] ±60	1800[a] ±240	8E-5 ±2E-5[b] [0.01]	8E-4 ±2E-4[b] [0.1]	4E-3 ±2E-3[b] [0.25]
Bentonite	2070[a] ±276	2070[a] ±276	2070[a] ±276	3E-3 ±4E-4[b] [0.2]	3E-3 ±4E-4[b] [0.2]	3E-3 ±4E-4[b] [0.2]
Sand-bentonite	1065[a] ±267	1065[a] ±267	1065[a] ±267	3E-3 ±5E-4[b] [0.08]	3E-3 ±5E-4[b] [0.08]	3E-3 ±5E-4[b] [0.08]
Sand	1855[a] ±265	1855[a] ±265	1855[a] ±265	2E-2 ±6E-3[b] [1.0]	2E-2 ±6E-3[b] [1.0]	2E-2 ±6E-3[b] [1.0]
Backfill	1890[a] ±270	1890[a] ±270	1890[a] ±270	2E-2 ±6E-3[d] [1.0]	2E-2 ±6E-3[d] [1.0]	2E-2 ±6E-3[d] [1.0]
Near-field rock fractures	2697[a] (2646 - 2699)	2697[a] (2646 - 2699)	2697[a] (2646 - 2699)	2E-6[e] (2E-5 – 3E-7)	2E-6[e] (2E-5 - 3E-7)	2E-6[e] (2E-5 - 3E-7)
Near-field rock matrix	2687[a] (2673 - 2697)	2687[a] (2673 - 2697)	2687[a] (2673 - 2697)	2E-6[c] (2E-5 – 3E-7)	2E-6[c] (2E-5 - 3E-7)	2E-6[c] (2E-5 - 3E-7)

[a] Assumes the following solid densities (kg m^{-3}): concrete = 2400 (Skagius et al., 1999); sand = 2650 (Deer et al., 1992); bentonite = 2760 (Nagra, 1994b); backfill, rock = 2700 (Krauskopf and Bird, 1995). Uncertainties are assumed to be those associated with porosity. [b] Höglund and Bengtsson (1991), but with repository evolutionary stages as defined in Section 1 of this report. Uncertainties are assumed to be those associated with porosity. [c] Skagius et al. (1999), but assuming a free diffusion coefficient (D_0) of 6×10^{-2} m^2 y^{-1}. See text for details. [d] Skagius et al., 1999. [e] Assumed identical to that for the rock matrix.

3 Sorption data

Sorption databases in the form of best estimate and pessimistic K_d values, have been provided for sorption of selected radioelements on the following substrates:

- porous concrete (waste matrix);
- structural concrete;
- bentonite;
- sand-bentonite (90%:10% mixture);
- sand;
- backfill (crushed rock);
- near-field rock fractures;
- near-field rock matrix;
- far-field rock fractures;
- far-field rock matrix.

The corresponding databases are shown in Table 3.1. All values are clearly referenced to a specific database or report, with the exception of those elements for which a chemical analogue was used.

The vaults have been subdivided according to different components of the Silo, BMA/BLA and BTF vaults, thereby accounting for different near-field barriers in each section of the repository. Best estimate values are taken from Stenhouse (Stenhouse, 2000). Pessimistic values provided for each element are either based on a K_d value provided in a similar database elsewhere, or are a reflection of the lack of data for a particular element. These (pessimistic) values are always equal to, or smaller than, the lowest corresponding database K_d. Thus, such values, in concert with sensitivity analysis, may be used to highlight those radioelements for which more experimental work is merited.

3.1 Sorption on Waste Matrix (Porous Concrete)

For those wastes immobilised in cement, K_d values are provided for sorption on cementitious material (porous concrete). Certain types of waste, e.g. ion exchange resins, are expected to provide additional immobilisation for the radionuclides they contain, but no credit has been given to this possibility.

Similarly, for those waste immobilised in bitumen, no credit for sorption is given to this matrix. Finally, no sorption is credited for those wastes not immobilised.

3.2 Sorption on Cementitious Materials

The bulk of the best estimate K_d values for cementitious materials have been taken from Savage et al. (Savage et al., 2000). Some elements for which K_d values are required, were not included in the original report, but are included in Table 3.1. Values for these elements were assigned by chemical analogy, *viz.*

- Fe: Ni used as chemical analogue;
- Co: Ni used as chemical analogue;
- Ru: Pd used as chemical analogue;
- Po: Pb/Sn used as chemical analogue.

Low (pessimistic) K_d values have been selected specifically for sensitivity analysis. The influence of different types of cement on sorption behaviour is discussed in Savage et al. (2000). Essentially, the conclusion in this report and elsewhere (Bradbury and Sarott, 1995; Krupka and Serne, 1998) is that the cement phases which dominate sorption are CSH phases which are common to all types of cement, at least during Stages I and II. Thus, identical K_d values are provided for sorption on different cements/concrete, so that differences in radionuclide transport through different cementitious materials will be governed only by differences in physical parameters (tortuosity, constrictivity, porosity; these parameters expressed through diffusivity) for each cement/concrete.

3.3 Sorption on Sand

Since sand consists primarily of silica, best estimate K_d values for sorption of radioelements on quartz have been used to compile this database. Most of these data were obtained from Stenhouse (Stenhouse, 1995). Note, however, that Bradbury and Sarott (1995) conservatively used K_d values for sorption on quartz/sand for Stage III in the evolution of cement, during which CSH phases were unstable, i.e. being dissolved.

3.4 Sorption on Compacted Bentonite and Sand-Bentonite

Compacted bentonite and sand-bentonite act as component barriers around different parts of the Silo section of the repository.

K_d values for sorption on compacted bentonite for the Safety Report 97 ('SR 97') are given in Andersson (1999) and these values and their sources (Yu and Neretnieks, 1997; Ochs, 1997) were reviewed by Stenhouse (2000). We also take into account the findings of Ochs (1997) who modelled the bentonite pore water composition when pore water was equilibrated with saline and freshwater groundwaters. His findings indicate that the influence of the groundwater composition is small relative to the effects of (natural) impurities in the bentonite. This conclusion is supported by the modelling conducted by Bruno et al. (1999). Thus, best estimate and pessimistic K_d values relate to reducing conditions and a saline groundwater.

The sand-bentonite barrier is assumed to consist of 10 % bentonite and 90 % sand (Appendix 2, SKI, 1994). The issue here is whether the extent of radioelement sorption is a 'composite K_d' for bentonite + sand (i.e. = 0.1 K_d compacted bentonite + 0.9 K_d sand), reflecting the reduced proportion of bentonite in the barrier. We believe that a factor of 10 reduction in K_d values for sorption on compacted bentonite will probably understimate the extent of sorption because not all sorption sites will be occupied. However, as a basis for developing the database, the composite approach is reasonable and conservative. This is also the approach taken by SKI (1994; Appendix 2) and Andersson (1999). Again, best estimate and pessimistic K_d values relate to reducing conditions and a saline groundwater.

3.5 Influence of Organic Complexants

The effect of organic complexants on radionuclide sorption behaviour is discussed in detail in Savage et al. (2000). The conclusion from this report is that, at the concentrations of organic complexants predicted in the SFR 1 repository, only degradation products of cellulose, specifically iso-saccharanic acid (ISA) would influence the sorption of certain elements, specifically actinides, lanthanides and transition elements. Note is also taken of the conclusions of a previous Working Group established by SKI to assess the impact of cellulose degradation products on sorption (SKI, 1994).

The calculational basis described in Bradbury and Sarott (1995) is used here to determine the estimated maximum ISA concentration in waste packages, and the associated sorption reduction factors for Pu.

For a cellulose loading of ~ 1 wt. % (BMA), the maximum *local* ISA concentration is estimated to be ~10^{-4} M, equivalent to a sorption reduction factor of ~ 500 (cf. 300 estimated in SKI, 1994). The elements affected, besides Pu, are Ac, Th, Am, and Cm, and, to a lesser extent, Pa, U and Np. Similarly, for a cellulose loading of ~ 0.1 wt. % (BTF and Silo), the maximum local ISA concentration is estimated to be ~10^{-5} M, equivalent to a sorption reduction factor of ~ 20 (cf. 30 estimated in SKI, 1994). The elements affected, besides Pu, are in this case only Ac, Th, Am, and Cm.

The above reduction factors are considered conservative and, for this reason, are taken into account in the best estimate and pessimistic K_d values for the cementitious waste conditioning matrix and grouting material, and, for other materials, only in the pessimistic K_d values.

3.6 Sorption on Near-Field and Far-Field Rock

Near-field and far-field rock are treated in a similar way as no major differences in minerals are expected between these two barriers.

The geology of the Forsmark area comprises two main types of rock: granite gneiss and sedimentary gneiss, both fine- to medium-grained. The predominant minerals of the fractures are calcite, chlorite, quartz, laumontite, biotite and clay minerals (SKI, 1984). In these respects, the geology of the Forsmark area is similar to that of SFL 3-5 (Andersson, 1999).

K_d values for sorption on the near-field rock *matrix* are taken from the K_d database for SR 97, taking account of the original values provided by Carbol and Engkvist (1997), the review of this work by Bruno et al. (1997) and the associated review by Stenhouse (2000).

Again, the nature of the near-field rock for the SFR 1 repository is similar to that for the SFL repository. Secondary minerals in *fractures* are assumed to contain higher sorbing minerals, e.g. a greater clay component, than those of the rock matrix. Here, the best estimate K_d values for fracture minerals are taken from Table 10 of Stenhouse (1995) since the reference mineralogy of the crystalline rock in Switzerland is qualitatively similar to that of the Swedish rock. In fact, these values are either the same as, or smaller than values compiled by Andersson (1996) for SITE-94, with one exception – the K_d value for I is taken from the latter reference. The pessimistic K_d values, however, are taken to be the same as those for the rock matrix, for the benefit of sensitivity analysis.

Pb was not included in the database of Carbol and Engkvist (1997) and a best estimate K_d value for this element is taken from Albinsson (1991).

In all cases (near-field and far-field rock; fractures and matrix), the interacting groundwater is assumed conservatively to be saline. For a few elements (Sr, Cs, Ra), higher K_d values might be expected in the case of a non-saline groundwater.

Table 3.1 Best estimate and pessimistic K_d values for sorption on different substrates (m^3/kg).

	Best Estimate and Pessimistic K_d Values (m^3/kg)														
	Silo: walls, bottom, lid			*Silo: porous concrete*			*Silo: compartment walls*			*Silo: moulds*			*Silo: conditioning cement*		
	I	***II***	***III***	***I***	***II***	***III***	***I***	***II***	***III***	***I***	***II***	***III***	***I***	***II***	***III***
C	0.5 ^{a} 0.01 ^{d}	0.5 ^{a} 0.01 ^{d}	0.01 ^{a} 0 ^{d}	0.5 ^{a} 0.01 ^{d}	0.5 ^{a} 0.01 ^{d}	0.01 ^{a} 0 ^{d}	0.5 ^{a} 0.01 ^{d}	0.5 ^{a} 0.01 ^{d}	0.01 ^{a} 0 ^{d}	0.5 ^{a} 0.01 ^{d}	0.5 ^{a} 0.01 ^{d}	0.01 ^{a} 0 ^{d}	0.5 ^{a} 0.01 ^{d}	0.5 ^{a} 0.01 ^{d}	0.01 ^{a} 0 ^{d}
Fe [=Ni]	0.1 0.01	0.1 0.01	0.01 0.001	0.1 0.01	0.1 0.01	0.01 0.001	0.1 0.01	0.1 0.01	0.01 0.001	0.1 0.01	0.1 0.01	0.01 0.001	0.1 0.01	0.1 0.01	0.01 0.001
Ni	0.1 ^{a} 0.01 ^{d}	0.1 ^{a} 0.01 ^{d}	0.01 ^{a} 0.001 ^{d}	0.1 ^{a} 0.01 ^{d}	0.1 ^{a} 0.01 ^{d}	0.01 ^{a} 0.001 ^{d}	0.1 ^{a} 0.01 ^{d}	0.1 ^{a} 0.01 ^{d}	0.01 ^{a} 0.001 ^{d}	0.1 ^{a} 0.01 ^{d}	0.1 ^{a} 0.01 ^{d}	0.01 ^{a} .001^{d}	0.1 ^{a} 0.01 ^{d}	0.1 ^{a} 0.01 ^{d}	0.01 ^{a} 0.001 ^{d}
Co [=Ni]	0.1 0.01	0.1 0.01	0.01 0.001	0.1 0.01	0.1 0.01	0.01 0.001	0.1 0.01	0.1 0.01	0.01 0.001	0.1 0.01	0.1 0.01	0.01 0.001	0.1 0.01	0.1 0.01	0.01 0.001
Sr	0.005 ^{a} 0.001^{b}	0.005 ^{a} 0.001^{b}	0.005 ^{a} 0.001^{b}	0.005 ^{a} 0.001^{b}	0.005 ^{a} 0.001^{b}	0.005 ^{a} 0.001^{b}	0.005 ^{a} 0.001^{b}	0.005 ^{a} 0.001^{b}	0.005 ^{a} 0.001^{b}	0.005 ^{a} 0.001^{b}	0.005 ^{a} 0.001^{b}	0.005 ^{a} 0.001^{b}	0.005 ^{a} 0.001^{b}	0.005 ^{a} 0.001^{b}	0.005 ^{a} 0.001^{b}
Nb	0.5 ^{a} 0.01 ^{d}	0.5 ^{a} 0.01 ^{d}	0.1 ^{a} 0.01^{d}	0.5 ^{a} 0.01 ^{d}	0.5 ^{a} 0.01 ^{d}	0.1 ^{a} 0.01^{d}	0.5 ^{a} 0.01 ^{d}	0.5 ^{a} 0.01 ^{d}	0.1 ^{a} 0.01^{d}	0.5 ^{a} 0.01 ^{d}	0.5 ^{a} 0.01 ^{d}	0.1 ^{a} 0.01^{d}	0.5 ^{a} 0.01 ^{d}	0.5 ^{a} 0.01 ^{d}	0.1 ^{a} 0.01^{d}
Tc (red.) Tc (ox.)	1 ^{a} 0.1 ^{d} 0.001^{b} 0 ^{c}	1 ^{a} 0.1 ^{d} 0.001^{b} 0 ^{c}	1 ^{a} 0.1 ^{d} 0 ^{b} ---	1 ^{a} 0.1 ^{d} 0.001^{b} 0 ^{c}	1 ^{a} 0.1 ^{d} 0.001^{b} 0 ^{c}	1 ^{a} 0.1 ^{d} 0 ^{b} ---	1 ^{a} 0.1 ^{d} 0.001^{b} 0 ^{c}	1 ^{a} 0.1 ^{d} 0.001^{b} 0 ^{c}	1 ^{a} 0.1 ^{d} 0 ^{b} ---	1 ^{a} 0.1 ^{d} 0.001^{b} 0 ^{c}	1 ^{a} 0.1 ^{d} 0.001^{b} 0 ^{c}	1 ^{a} 0.1 ^{d} 0 ^{b} ---	1 ^{a} 0.1 ^{d} 0.001^{b} 0 ^{c}	1 ^{a} 0.1 ^{d} 0.001^{b} 0 ^{c}	1 ^{a} 0.1 ^{d} 0 ^{b} ---
Ru [=Pd]	0.5 ^{a} 0.001^{b}	0.5 ^{a} 0.001^{b}	0.1 ^{a} 0.001^{b}	0.5 ^{a} 0.001^{b}	0.5 ^{a} 0.001^{b}	0.1 ^{a} 0.001^{b}	0.5 ^{a} 0.001^{b}	0.5 ^{a} 0.001^{b}	0.1 ^{a} 0.001^{b}	0.5 ^{a} 0.001^{b}	0.5 ^{a} 0.001^{b}	0.1 ^{a} 0.001^{b}	0.5 ^{a} 0.001^{b}	0.5 ^{a} 0.001^{b}	0.1 ^{a} 0.001^{b}
I	0.02 ^{a} 0 ^{d}	0.02 ^{a} 0 ^{d}	0.01 ^{a} 0 ^{d}	0.02 ^{a} 0 ^{d}	0.02 ^{a} 0 ^{d}	0.01 ^{a} 0 ^{d}	0.02 ^{a} 0 ^{d}	0.02 ^{a} 0 ^{d}	0.01 ^{a} 0 ^{d}	0.02 ^{a} 0 ^{d}	0.02 ^{a} 0 ^{d}	0.01 ^{a} 0 ^{d}	0.02 ^{a} 0 ^{d}	0.02 ^{a} 0 ^{d}	0.01 ^{a} 0 ^{d}
Cs	0.001 ^{a} 0.0005^{d}	0.001 ^{a} 0.0005^{d}	0.005 ^{a} 0.001 ^{d}	0.001 ^{a} 0.0005^{d}	0.001 ^{a} 0.0005^{d}	0.005 ^{a} 0.001 ^{d}	0.001 ^{a} 0.0005^{d}	0.001 ^{a} 0.0005^{d}	0.005 ^{a} 0.001 ^{d}	0.001 ^{a} 0.0005^{d}	0.001 ^{a} 0.0005^{d}	0.005 ^{a} 0.001^{d}	0.001 ^{a} 0.0005^{d}	0.001 ^{a} 0.0005^{d}	0.005 ^{a} 0.001 ^{d}
Pb	0.5 ^{a} 0.05 ^{b}	0.5 ^{a} 0.05 ^{b}	0.1 ^{a} 0.01 ^{d}	0.5 ^{a} 0.05 ^{b}	0.5 ^{a} 0.05 ^{b}	0.1 ^{a} 0.01 ^{d}	0.5 ^{a} 0.05 ^{b}	0.5 ^{a} 0.05 ^{b}	0.1 ^{a} 0.01 ^{d}	0.5 ^{a} 0.05 ^{b}	0.5 ^{a} 0.05 ^{b}	0.1 ^{a} 0.01^{d}	0.5 ^{a} 0.05 ^{b}	0.5 ^{a} 0.05 ^{b}	0.1 ^{a} 0.01^{d}
Po [=Pb]	0.5 ^{a} 0.05 ^{b}	0.5 ^{a} 0.05 ^{b}	0.1 ^{a} 0.01 ^{d}	0.5 ^{a} 0.05 ^{b}	0.5 ^{a} 0.05 ^{b}	0.1 ^{a} 0.01 ^{d}	0.5 ^{a} 0.05 ^{b}	0.5 ^{a} 0.05 ^{b}	0.1 ^{a} 0.01 ^{d}	0.5 ^{a} 0.05 ^{b}	0.5 ^{a} 0.05 ^{b}	0.1 ^{a} 0.01^{d}	0.5 ^{a} 0.05 ^{b}	0.5 ^{a} 0.05 ^{b}	0.1 ^{a} 0.01^{d}

[a] Table 2.4, Savage et al. (2000); [b] Table 4, Bradbury and Sarott (1995); [c] Table 5.1, Krupka and Serne (1999); [d] arbitrary value for sensitivity analysis; [e] Table 9-3, Vieno and Nordman, 1998.

Table 3.1 (continued) Best estimate and pessimistic K_d values for sorption on different substrates (m^3/kg).

	Best Estimate and Pessimistic K_d Values (m^3/kg)														
	Silo: walls, bottom, lid			*Silo: porous concrete*			*Silo: compartment walls*			*Silo: moulds*			*Silo: conditioning cement*		
	I	***II***	***III***	***I***	***II***	***III***	***I***	***II***	***III***	***I***	***II***	***III***	***I***	***II***	***III***
Pu	5^{a} 0.005^{p}	5^{a} 0.005^{p}	1^{a} 0.005^{p}	0.25^{q} 0.005^{p}	0.25^{q} 0.005^{p}	0.05^{q} 0.005^{p}	5^{a} 0.005^{p}	5^{a} 0.005^{p}	1^{a} 0.005^{p}	5^{a} 0.005^{p}	5^{a} 0.005^{p}	1^{a} 0.005^{p}	0.25^{q} 0.005^{p}	0.25^{q} 0.005^{p}	0.05^{q} 0.005^{p}
Ra	0.05^{a} 0.005^{d}	0.05^{a} 0.005^{d}	0.05^{a} 0.005^{d}	0.05^{a} 0.005^{d}	0.05^{a} 0.005^{d}	0.05^{a} 0.005^{d}	0.05^{a} 0.005^{d}	0.05^{a} 0.005^{d}	0.05^{a} 0.005^{d}	0.05^{a} 0.005^{d}	0.05^{a} 0.005^{d}	0.05^{a} 0.005^{d}	0.05^{a} 0.005^{d}	0.05^{a} 0.005^{d}	0.05^{a} 0.005^{d}
Ac	5^{a} 0.0025^{t}	5^{a} 0.0025^{t}	1^{a} 0.0025^{t}	0.25^{q} 0.0025^{t}	0.25^{q} 0.0025^{t}	0.05^{q} 0.005^{t}	5^{a} 0.0025^{p}	5^{a} 0.0025^{p}	1^{a} 0.0025^{p}	5^{a} 0.0025^{p}	5^{a} 0.0025^{p}	1^{a} 0.0025^{p}	0.25^{q} 0.0025^{p}	0.25^{q} 0.0025^{p}	0.05^{q} 0.0025^{p}
Th	5^{a} 0.005^{p}	5^{a} 0.005^{p}	1^{a} 0.005^{p}	0.25^{q} 0.005^{p}	0.25^{q} 0.005^{p}	0.05^{q} 0.005^{p}	5^{a} 0.005^{p}	5^{a} 0.005^{p}	1^{a} 0.005^{p}	5^{a} 0.005^{p}	5^{a} 0.005^{p}	1^{a} 0.005^{p}	0.25^{q} 0.005^{p}	0.25^{q} 0.005^{p}	0.05^{q} 0.005^{p}
Pa	0.5^{a} 0.1^{d}	0.5^{a} 0.1^{d}	0.1^{a} 0.01^{d}	0.5^{a} 0.1^{d}	0.5^{a} 0.1^{d}	0.1^{a} 0.01^{d}	0.5^{a} 0.1^{d}	0.5^{a} 0.1^{d}	0.1^{a} 0.01^{d}	0.5^{a} 0.1^{d}	0.5^{a} 0.1^{d}	0.1^{a} 0.01^{d}	0.5^{a} 0.1^{d}	0.5^{a} 0.1^{d}	0.1^{a} 0.01^{d}
U (red.) U (ox.)	5^{a} 0.1^{d} 1^{c} 0.01^{d}	5^{a} 0.1^{d} 1^{c} 0.01^{d}	1^{a} 0.1^{d} 0.1^{c} 0.01^{d}	5^{a} 0.1^{d} 1^{c} 0.01^{d}	5^{a} 0.1^{d} 1^{c} 0.01^{d}	1^{a} 0.1^{d} 0.1^{c} 0.01^{d}	5^{a} 0.1^{d} 1^{c} 0.01^{d}	5^{a} 0.1^{d} 1^{c} 0.01^{d}	1^{a} 0.1^{d} 0.1^{c} 0.01^{d}	5^{a} 0.1^{d} 1^{c} 0.01^{d}	5^{a} 0.1^{d} 1^{c} 0.01^{d}	1^{a} 0.1^{d} 0.1^{c} 0.01^{d}	5^{a} 0.1^{d} 1^{c} 0.01^{d}	5^{a} 0.1^{d} 1^{c} 0.01^{d}	1^{a} 0.1^{d} 0.1^{c} 0.01^{d}
Np (red.) Np (ox.)	5^{a} 0.1^{d} 2^{c} 0.01^{d}	5^{a} 0.1^{d} 2^{c} 0.01^{d}	1^{a} 0.1^{d} 0.1^{b} 0.01^{d}	5^{a} 0.1^{d} 2^{c} 0.01^{d}	5^{a} 0.1^{d} 2^{c} 0.01^{d}	1^{a} 0.1^{d} 0.1^{b} 0.01^{d}	5^{a} 0.1^{d} 2^{c} 0.01^{d}	5^{a} 0.1^{d} 2^{c} 0.01^{d}	1^{a} 0.1^{d} 0.1^{b} 0.01^{d}	5^{a} 0.1^{d} 2^{c} 0.01^{d}	5^{a} 0.1^{d} 2^{c} 0.01^{d}	1^{a} 0.1^{d} 0.1^{b} 0.01^{d}	5^{a} 0.1^{d} 2^{c} 0.01^{d}	5^{a} 0.1^{d} 2^{c} 0.01^{d}	1^{a} 0.1^{d} 0.1^{b} 0.01^{d}
Am	5^{a} 0.0025^{p}	5^{a} 0.0025^{p}	1^{a} 0.0025^{p}	0.25^{q} 0.0025^{p}	0.25^{q} 0.0025^{p}	0.05^{q} 0.0025^{p}	5^{a} 0.0025^{p}	5^{a} 0.0025^{p}	1^{a} 0.0025^{p}	5^{a} 0.0025^{p}	5^{a} 0.0025^{p}	1^{a} 0.0025^{p}	0.25^{q} 0.0025^{p}	0.25^{q} 0.0025^{p}	0.05^{q} 0.0025^{p}
Cm	5^{a} 0.0025^{p}	5^{a} 0.0025^{p}	1^{a} 0.0025^{p}	0.25^{q} 0.0025^{p}	0.25^{q} 0.0025^{p}	0.05^{q} 0.0025^{p}	5^{a} 0.0025^{p}	5^{a} 0.0025^{p}	1^{a} 0.0025^{p}	5^{a} 0.0025^{p}	5^{a} 0.0025^{p}	1^{a} 0.0025^{p}	0.25^{q} 0.0025^{p}	0.25^{q} 0.0025^{p}	0.05^{q} 0.0025^{p}

[a] : Table 2.4, Savage et al. (2000); [c]: Table 5.1, Krupka and Serne (1999); [d]: arbitrary value for sensitivity analysis; [e]: Table 9-3, Vieno and Nordman (1998);
[m]: Effect of organics: sorption reduction factors for Pu (Table 5) and certain other elements relative to Pu (Table 9), Bradbury and Sarott (1995); [p]: = e + m; [q]: = a + m.

Table 3.1 (continued) Best estimate and pessimistic K_d values for sorption on different substrates (m^3/kg).

	Best Estimate and Pessimistic K_d Values (m^3/kg)														
	BMA: construction concrete			*BMA: moulds*			*BTF: construction concrete*			*BTF: moulds*			*BTF: porous concrete*		
	I	***II***	***III***	***I***	***II***	***III***	***I***	***II***	***III***	***I***	***II***	***III***	***I***	***II***	***III***
C	0.5^{a} 0.01^{d}	0.5^{a} 0.01^{d}	0.01^{a} 0^{d}	0.5^{a} 0.01^{d}	0.5^{a} 0.01^{d}	0.01^{a} 0^{d}	0.5^{a} 0.01^{d}	0.5^{a} 0.01^{d}	0.01^{a} 0^{d}	0.5^{a} 0.01^{d}	0.5^{a} 0.01^{d}	0.01^{a} 0^{d}	0.5^{a} 0.01^{d}	0.5^{a} 0.01^{d}	0.01^{a} 0^{d}
Fe [=Ni]	0.1 0.01	0.1 0.01	0.01 0.001	0.1 0.01	0.1 0.01	0.01 0.001	0.1 0.01	0.1 0.01	0.01 0.001	0.1 0.01	0.1 0.01	0.01 0.001	0.1 0.01	0.1 0.01	0.01 0.001
Ni	0.1^{a} 0.01^{d}	0.1^{a} 0.01^{d}	0.01^{a} 0.001^{d}	0.1^{a} 0.01^{d}	0.1^{a} 0.01^{d}	0.01^{a} 0.001^{d}	0.1^{a} 0.01^{d}	0.1^{a} 0.01^{d}	0.01^{a} 0.001^{d}	0.1^{a} 0.01^{d}	0.1^{a} 0.01^{d}	0.01^{a} 0.001^{d}	0.1^{a} 0.01^{d}	0.1^{a} 0.01^{d}	0.01^{a} 0.001^{d}
Co [=Ni]	0.1 0.01	0.1 0.01	0.01 0.001	0.1 0.01	0.1 0.01	0.01 0.001	0.1 0.01	0.1 0.01	0.01 0.001	0.1 0.01	0.1 0.01	0.01 0.001	0.1 0.01	0.1 0.01	0.01 0.001
Sr	0.005^{a} 0.001^{b}	0.005^{a} 0.001^{b}	0.005^{a} 0.001^{b}	0.005^{a} 0.001^{b}	0.005^{a} 0.001^{b}	0.005^{a} 0.001^{b}	0.005^{a} 0.001^{b}	0.005^{a} 0.001^{b}	0.005^{a} 0.001^{b}	0.005^{a} 0.001^{b}	0.005^{a} 0.001^{b}	0.005^{a} 0.001^{b}	0.005^{a} 0.001^{b}	0.005^{a} 0.001^{b}	0.005^{a} 0.001^{b}
Nb	0.5^{a} 0.01^{d}	0.5^{a} 0.01^{d}	0.1^{a} 0.01^{d}	0.5^{a} 0.01^{d}	0.5^{a} 0.01^{d}	0.1^{a} 0.01^{d}	0.5^{a} 0.01^{d}	0.5^{a} 0.01^{d}	0.1^{a} 0.01^{d}	0.5^{a} 0.01^{d}	0.5^{a} 0.01^{d}	0.1^{a} 0.01^{d}	0.5^{a} 0.01^{d}	0.5^{a} 0.01^{d}	0.1^{a} 0.01^{d}
Tc (red.) Tc (ox.)	1^{a} 0.1^{d} 0.001^{b} 0^{c}	1^{a} 0.1^{d} 0.001^{b} 0^{c}	1^{a} 0.1^{d} 0^{b} ---	1^{a} 0.1^{d} 0.001^{b} 0^{c}	1^{a} 0.1^{d} 0.001^{b} 0^{c}	1^{a} 0.1^{d} 0^{b} ---	1^{a} 0.1^{d} 0.001^{b} 0^{c}	1^{a} 0.1^{d} 0.001^{b} 0^{c}	1^{a} 0.1^{d} 0^{b} ---	1^{a} 0.1^{d} 0.001^{b} 0^{c}	1^{a} 0.1^{d} 0.001^{b} 0^{c}	1^{a} 0.1^{d} 0^{b} ---	1^{a} 0.1^{d} 0.001^{b} 0^{c}	1^{a} 0.1^{d} 0.001^{b} 0^{c}	1^{a} 0.1^{d} 0^{b} ---
Ru [=Pd]	0.5^{a} 0.001^{b}	0.5^{a} 0.001^{b}	0.1^{a} 0.001^{b}	0.5^{a} 0.001^{b}	0.5^{a} 0.001^{b}	0.1^{a} 0.001^{b}	0.5^{a} 0.001^{b}	0.5^{a} 0.001^{b}	0.1^{a} 0.001^{b}	0.5^{a} 0.001^{b}	0.5^{a} 0.001^{b}	0.1^{a} 0.001^{b}	0.5^{a} 0.001^{b}	0.5^{a} 0.001^{b}	0.1^{a} 0.001^{b}
I	0.02^{a} 0^{d}	0.02^{a} 0^{d}	0.01^{a} 0^{d}	0.02^{a} 0^{d}	0.02^{a} 0^{d}	0.01^{a} 0^{d}	0.02^{a} 0^{d}	0.02^{a} 0^{d}	0.01^{a} 0^{d}	0.02^{a} 0^{d}	0.02^{a} 0^{d}	0.01^{a} 0^{d}	0.02^{a} 0^{d}	0.02^{a} 0^{d}	0.01^{a} 0^{d}
Cs	0.001^{a} 0.0005^{d}	0.001^{a} 0.0005^{d}	0.005^{a} 0.001^{d}	0.001^{a} 0.0005^{d}	0.001^{a} 0.0005^{d}	0.005^{a} 0.001^{d}	0.001^{a} 0.0005^{d}	0.001^{a} 0.0005^{d}	0.005^{a} 0.001^{d}	0.001^{a} 0.0005^{d}	0.001^{a} 0.0005^{d}	0.005^{a} 0.001^{d}	0.001^{a} 0.0005^{d}	0.001^{a} 0.0005^{d}	0.005^{a} 0.001^{d}
Pb	0.5^{a} 0.05^{b}	0.5^{a} 0.05^{b}	0.1^{a} 0.01^{d}	0.5^{a} 0.05^{b}	0.5^{a} 0.05^{b}	0.1^{a} 0.01^{d}	0.5^{a} 0.05^{b}	0.5^{a} 0.05^{b}	0.1^{a} 0.01^{d}	0.5^{a} 0.05^{b}	0.5^{a} 0.05^{b}	0.1^{a} 0.01^{d}	0.5^{a} 0.05^{b}	0.5^{a} 0.05^{b}	0.1^{a} 0.01^{d}
Po [=Pb]	0.5^{a} 0.05^{b}	0.5^{a} 0.05^{b}	0.1^{a} 0.01^{d}	0.5^{a} 0.05^{b}	0.5^{a} 0.05^{b}	0.1^{a} 0.01^{d}	0.5^{a} 0.05^{b}	0.5^{a} 0.05^{b}	0.1^{a} 0.01^{d}	0.5^{a} 0.05^{b}	0.5^{a} 0.05^{b}	0.1^{a} 0.01^{d}	0.5^{a} 0.05^{b}	0.5^{a} 0.05^{b}	0.1^{a} 0.01^{d}

[a] : Table 2.4, Savage et al. (2000); [b]: Table 4, Bradbury and Sarott (1995); [c]: Table 5.1, Krupka and Serne (1999); [d]: arbitrary value for sensitivity analysis;
[e]: Table 9-3, Vieno and Nordman (1998).

Table 3.1 (continued) Best estimate and pessimistic K_d values for sorption on different substrates (m^3/kg).

	Best Estimate and Pessimistic K_d Values (m^3/kg)														
	BMA: construction concrete			*BMA: moulds*			*BTF: construction concrete*			*BTF: moulds*			*BTF: porous concrete*		
	I	***II***	***III***	***I***	***II***	***III***	***I***	***II***	***III***	***I***	***II***	***III***	***I***	***II***	***III***
Pu	5^{a} 2E-04^{p}	5^{a} 2E-04^{p}	1^{a} 2E-04^{p}	5^{a} 2E-04^{p}	5^{a} 2E-04^{p}	1^{a} 2E-04^{p}	5^{a} 0.005^{p}	5^{a} 0.005^{p}	1^{a} 0.005^{p}	5^{a} 0.005^{p}	5^{a} 0.005^{p}	1^{a} 0.005^{p}	0.25^{q} 0.005^{p}	0.25^{q} 0.005^{p}	0.05^{q} 0.005^{p}
Ra	0.05^{a} 0.005^{d}	0.05^{a} 0.005^{d}	0.05^{a} 0.005^{d}	0.05^{a} 0.005^{d}	0.05^{a} 0.005^{d}	0.05^{a} .005^{d}	0.05^{a} 0.005^{d}	0.05^{a} 0.005^{d}	0.05^{a} 0.005^{d}	0.05^{a} 0.005^{d}	0.05^{a} 0.005^{d}	0.05^{a} .005^{d}	0.05^{a} 0.005^{d}	0.05^{a} 0.005^{d}	0.05^{a} 0.005^{d}
Ac	5^{a} 1E-04^{v}	5^{a} 1E-04^{v}	1^{a} 1E-04^{v}	5^{a} 1E-04^{v}	5^{a} 1E-04^{v}	1^{a} 1E-04^{v}	5^{a} 0.0025^{v}	5^{a} 0.0025^{v}	1^{a} 0.0025^{v}	5^{a} 0.0025^{v}	5^{a} 0.0025^{v}	1^{a} 0.0025^{v}	0.25^{q} 0.0025^{v}	0.25^{q} 0.0025^{v}	0.05^{q} 0.0025^{v}
Th	5^{a} 2E-04^{v}	5^{a} 2E-04^{v}	1^{a} 2E-04^{v}	5^{a} 2E-04^{v}	5^{a} 2E-04^{v}	1^{a} 2E-04^{v}	5^{a} 0.005^{v}	5^{a} 0.005^{v}	1^{a} 0.005^{v}	5^{a} 0.005^{v}	5^{a} 0.005^{v}	1^{a} 0.005^{v}	0.25^{q} 0.005^{v}	0.25^{q} 0.005^{v}	0.05^{q} 0.005^{v}
Pa	0.5^{a} 0.04^{v}	0.5^{a} 0.04^{v}	0.1^{a} 0.04^{v}	0.5^{a} 0.04^{v}	0.5^{a} 0.04^{v}	0.1^{a} 0.04^{v}	0.5^{a} 0.1^{d}	0.5^{a} 0.1^{d}	0.1^{a} 0.01^{d}	0.5^{a} 0.1^{d}	0.5^{a} 0.1^{d}	0.1^{a} 0.01^{d}	0.5^{a} 0.1^{d}	0.5^{a} 0.1^{d}	0.1^{a} 0.01^{d}
U (red.) U (ox.)	5^{a} 0.04^{v} 1^{c} 0.004^{v}	5^{a} 0.04^{v} 1^{c} 0.004^{v}	1^{a} 0.04^{v} 0.1^{c} 0.004^{v}	5^{a} 0.04^{v} 1^{c} 0.004^{v}	5^{a} 0.04^{v} 1^{c} 0.004^{v}	1^{a} 0.04^{v} 0.1^{c} 0.004^{v}	5^{a} 0.1^{d} 1^{c} 0.01^{d}	5^{a} 0.1^{d} 1^{c} 0.01^{d}	1^{a} 0.1^{d} 0.1^{c} 0.01^{d}	5^{a} 0.1^{d} 1^{c} 0.01^{d}	5^{a} 0.1^{d} 1^{c} 0.01^{d}	1^{a} 0.1^{d} 0.1^{c} 0.01^{d}	5^{a} 0.1^{d} 1^{c} 0.01^{d}	5^{a} 0.1^{d} 1^{c} 0.01^{d}	1^{a} 0.1^{d} 0.1^{c} 0.01^{d}
Np (red.) Np (ox.)	5^{a} 0.04^{v} 2^{c} 0.004^{v}	5^{a} 0.04^{v} 2^{c} 0.004^{v}	1^{a} 0.04^{v} 0.2^{c} 0.004^{v}	5^{a} 0.04^{v} 2^{c} 0.004^{v}	5^{a} 0.04^{v} 2^{c} 0.004^{v}	1^{a} 0.04^{v} 0.2^{c} 0.004^{v}	5^{a} 0.1^{d} 2^{c} 0.01^{d}	5^{a} 0.1^{d} 2^{c} 0.01^{d}	1^{a} 0.1^{d} 0.2^{c} 0.01^{d}	5^{a} 0.1^{d} 2^{c} 0.01^{d}	5^{a} 0.1^{d} 2^{c} 0.01^{d}	1^{a} 0.1^{d} 0.2^{c} 0.01^{d}	5^{a} 0.1^{d} 2^{c} 0.01^{d}	5^{a} 0.1^{d} 2^{c} 0.01^{d}	1^{a} 0.1^{d} 0.2^{c} 0.01^{d}
Am	5^{a} 1E-04^{p}	5^{a} 1E-04^{p}	1^{a} 1E-04^{p}	5^{a} 1E-04^{p}	5^{a} 1E-04^{p}	1^{a} 1E-04^{p}	5^{a} 0.0025^{p}	5^{a} 0.0025^{p}	1^{a} 0.0025^{p}	5^{a} 0.0025^{p}	5^{a} 0.0025^{p}	1^{a} 0.0025^{p}	0.25^{q} 0.0025^{p}	0.25^{q} 0.0025^{p}	0.05^{q} 0.0025^{p}
Cm	5^{a} 1E-04^{p}	5^{a} 1E-04^{p}	1^{a} 1E-04^{p}	5^{a} 1E-04^{p}	5^{a} 1E-04^{p}	1^{a} 1E-04^{p}	5^{a} 0.0025^{p}	5^{a} 0.0025^{p}	1^{a} 0.0025^{p}	5^{a} 0.0025^{p}	5^{a} 0.0025^{p}	1^{a} 0.0025^{p}	0.25^{q} 0.0025^{p}	0.25^{q} 0.0025^{p}	0.05^{q} 0.0025^{p}

[a] Table 2.4, Savage et al. (2000); [b] Table 4, Bradbury and Sarott (1995); [c] Table 5.1, Krupka and Serne (1999); [d] arbitrary value for sensitivity analysis;
[e] Table 9-3, Vieno and Nordman (1998); [m]: Effect of organics: sorption reduction factors for Pu (Table 5) and for certain other elements (Table 9), Bradbury and Sarott (1995);
[p]: = e + m; [q]: = a + m; [v]: = d + m; [w]:= c + m.

Table 3.1 (continued) Best estimate and pessimistic K_d values for sorption on different substrates (m^3/kg).

	Best Estimate and Pessimistic K_d Values (m^3/kg)														
	Waste matrix [Silo, BMA, BTF] (porous concrete)			*Structural concrete*			*Bentonite*			*Sand-Bentonite (90%:10%)*			*Sand*		
	I	***II***	***III***	***I***	***II***	***III***	***I***	***II***	***III***	***I***	***II***	***III***	***I***	***II***	***III***
C	0.5^{a} 0.01^{d}	0.5^{a} 0.01^{d}	0.01^{a} 0^{d}	0.5^{a} 0.01^{d}	0.5^{a} 0.01^{d}	0.01^{a} 0^{d}	0^{g} ---	0^{g} ---	0^{g} ---	0^{h} ---	0^{h} ---	0^{h} ---	0^{f} ---	0^{f} ---	0^{f} ---
Fe [=Ni]	0.1 0.01	0.1 0.01	0.01 0.001	0.1 0.01	0.1 0.01	0.01 0.001	0.1 0.02	0.1 0.02	0.1 0.02	0.05 0.003	0.05 0.003	0.05 0.003	0.04 0.001	0.04 0.001	0.04 0.001
Ni	0.1^{a} 0.01^{d}	0.1^{a} 0.01^{d}	0.01^{a} 0.001^{d}	0.1^{a} 0.01^{d}	0.1^{a} 0.01^{d}	0.01^{a} 0.001^{d}	0.1^{g} 0.02^{g}	0.1^{g} 0.02^{g}	0.1^{g} 0.02^{g}	0.05^{h} 0.003^{h}	0.05^{h} 0.003^{h}	0.05^{h} 0.003^{h}	0.04^{f} 0.001^{d}	0.04^{f} 0.001^{d}	0.04^{f} 0.001^{d}
Co [=Ni]	0.1 0.01	0.1 0.01	0.01 0.001	0.1 0.01	0.1 0.01	0.01 0.001	0.1 0.02	0.1 0.02	0.1 0.02	0.05 0.003	0.05 0.003	0.05 0.003	0.04 0.001	0.04 0.001	0.04 0.001
Sr	0.005^{a} 0.001^{b}	0.005^{a} 0.001^{b}	0.005^{a} 0.001^{b}	0.005^{a} 0.001^{b}	0.005^{a} 0.001^{b}	0.005^{a} 0.001^{b}	0.01^{g} 0.001^{g}	0.01^{g} 0.001^{g}	0.01^{g} 0.001^{g}	0.002^{h} 0.0002^{h}	0.002^{h} 0.0002^{h}	0.002^{h} 0.0002^{h}	0.001^{f} 0.0001^{d}	0.001^{f} 0.0001^{d}	0.001^{f} 0.0001^{d}
Nb	0.5^{a} 0.01^{d}	0.5^{a} 0.01^{d}	0.1^{a} 0.01^{d}	0.5^{a} 0.01^{d}	0.5^{a} 0.01^{d}	0.1^{a} 0.01^{d}	0.2^{g} 0^{g}	0.2^{g} 0^{g}	0.2^{g} 0^{g}	0.065^{h} 0^{h}	0.065^{h} 0^{h}	0.065^{h} 0^{h}	0.05^{f} 0^{d}	0.05^{f} 0^{d}	0.05^{f} 0^{d}
Tc (red.) Tc (ox.)	1^{a} 0.1^{d} 0.001^{b} 0^{c}	1^{a} 0.1^{d} 0.001^{b} 0^{c}	1^{a} 0.1^{d} 0^{b} ---	1^{a} 0.1^{d} 0.001^{b} 0^{c}	1^{a} 0.1^{d} 0.001^{b} 0^{c}	1^{a} 0.1^{d} 0^{b} ---	0.1^{g} 0.01^{g} 0^{f} ---	0.1^{g} 0.01^{g} 0^{f} ---	0.1^{g} 0.01^{g} 0^{f} ---	0.06^{h} 0.01^{h} 0^{h} ---	0.06^{h} 0.01^{h} 0^{h} ---	0.06^{h} 0.01^{h} 0^{h} ---	0.05^{f} 0.01^{f} 0^{f} ---	0.05^{f} 0.01^{f} 0^{f} ---	0.05^{f} 0.01^{f} 0^{f} ---
Ru [=Pd]	0.5^{a} 0.001^{b}	0.5^{a} 0.001^{b}	0.1^{a} 0.001^{b}	0.5^{a} 0.001^{b}	0.5^{a} 0.001^{b}	0.1^{a} 0.001^{b}	0.01^{g} 0^{g}	0.01^{g} 0^{g}	0.01^{g} 0^{g}	0.05^{h} 0^{h}	0.05^{h} 0^{h}	0.05^{h} 0^{h}	0.05^{f} 0^{d}	0.05^{f} 0^{d}	0.05^{f} 0^{d}
I	0.02^{a} 0^{d}	0.02^{a} 0^{d}	0.01^{a} 0^{d}	0.02^{a} 0^{d}	0.02^{a} 0^{d}	0.01^{a} 0^{d}	0^{g} ---	0^{g} ---	0^{g} ---	0^{h} ---	0^{h} ---	0^{h} ---	0^{f} ---	0^{f} ---	0^{f} ---
Cs	0.001^{a} 0.0001^{d}	0.001^{a} 0.0001^{d}	0.005^{a} 0.001^{d}	0.001^{a} 0.0001^{d}	0.001^{a} 0.0001^{d}	0.005^{a} 0.001^{d}	0.05^{g} 0.005^{g}	0.05^{g} 0.005^{g}	0.05^{g} 0.005^{g}	0.006^{h} 0.0006^{h}	0.006^{h} 0.0006^{h}	0.006^{h} 0.0006^{h}	0.001^{f} 0.0001^{d}	0.001^{f} 0.0001^{d}	0.001^{f} 0.0001^{d}
Pb	0.5^{a} 0.05^{b}	0.5^{a} 0.05^{b}	0.1^{a} 0.01^{d}	0.5^{a} 0.05^{b}	0.5^{a} 0.05^{b}	0.1^{a} 0.01^{d}	0.5^{g} 0^{g}	0.5^{g} 0^{g}	0.5^{g} 0^{g}	0.1^{h} 0^{h}	0.1^{h} 0^{h}	0.1^{h} 0^{h}	0.05^{f} 0^{d}	0.05^{f} 0^{d}	0.05^{f} 0^{d}
Po [=Pb]	0.5 0.05	0.5 0.05	0.1 0.01	0.5 0.05	0.5 0.05	0.1 0.01	0.5 0	0.5 0	0.5 0	0.1 0	0.1 0	0.1 0	0.05 0	0.05 0	0.05 0

[a] Table 2.4, Savage et al. (2000); [b] Table 4, Bradbury and Sarott (1995); [c] Table 5.1, Krupka and Serne (1999); [d] arbitrary value for sensitivity analysis; [e] Table 9-3, Vieno and Nordman (1998); [f]: Appendix B, Stenhouse (1995); [g]: Tables A.2.3.2 (compacted bentonite), Anderson (1999);[h]: = 0.9*K_d (sand) + 0.1*K_d (compacted bentonite).

Table 3.1 (continued) Best estimate and pessimistic K_d values for sorption on different substrates (m^3/kg).

	Best Estimate and Pessimistic K_d Values (m^3/kg)														
	Waste matrix [Silo, BTF] (porous concrete			*Structural concrete*			*Bentonite*			*Sand-Bentonite (90%:10%)*			*Sand*		
	I	***II***	***III***	***I***	***II***	***III***	***I***	***II***	***III***	***I***	***II***	***III***	***I***	***II***	***III***
Pu	0.25^{q} 0.005^{p}	0.25^{q} 0.005^{p}	0.05^{q} 0.005^{p}	5^{a} 0.005^{p}	5^{a} 0.005^{p}	1^{a} 0.005^{p}	3^{g} 0.05^{r}	3^{g} 0.05^{r}	3^{g} 0.05^{r}	0.75^{h} 0.01^{s}	0.75^{h} 0.01^{s}	0.75^{h} 0.01^{s}	0.5^{f} 0.005^{t}	0.5^{f} 0.005^{t}	0.5^{f} 0.005^{t}
Ra	0.05^{a} 0.005^{d}	0.05^{a} 0.005^{d}	0.05^{a} 0.005^{d}	0.05^{a} 0.005^{d}	0.05^{a} 0.005^{d}	0.05^{a} 0.005^{d}	0.01^{g} 0.001^{g}	0.01^{g} 0.001^{g}	0.01^{g} 0.001^{g}	0.004^{h} 0.0006^{h}	0.004^{h} 0.0006^{h}	0.004^{h} 0.0006^{h}	0.003^{f} 0.0005^{d}	0.003^{f} 0.0005^{d}	0.003^{f} 0.0005^{d}
Ac [=Am]	0.25^{q} 0.0025^{p}	0.25^{q} 0.0025^{p}	0.05^{q} 0.0025^{p}	5^{a} 0.0025^{p}	5^{a} 0.0025^{p}	1^{a} 0.0025^{p}	3 0.05	3 0.05	3 0.05	1^{h} 0.005^{h}	1^{h} 0.005^{h}	1^{h} 0.005^{h}	1^{f} $5E\text{-}04^{v}$	1^{f} $5E\text{-}04^{v}$	1^{f} $5E\text{-}04^{v}$
Th	0.25^{q} 0.005^{v}	0.25^{q} 0.005^{v}	0.05^{q} 0.005^{v}	5^{a} 0.005^{v}	5^{a} 0.005^{v}	1^{a} 0.005^{v}	3^{g} 0.005^{r}	3^{g} 0.005^{r}	3^{g} 0.005^{r}	1^{h} 0.001^{w}	1^{h} 0.001^{w}	1^{h} 0.001^{w}	1^{f} $5E\text{-}04^{v}$	1^{f} $5E\text{-}04^{v}$	1^{f} $5E\text{-}04^{v}$
Pa	0.5^{a} 0.1^{d}	0.5^{a} 0.1^{d}	0.1^{a} 0.01^{d}	0.5^{a} 0.1^{d}	0.5^{a} 0.1^{d}	0.1^{a} 0.01^{d}	0.3^{g} 0.001^{g}	0.3^{g} 0.001^{g}	0.3^{g} 0.001^{g}	0.1^{h} 0.009^{h}	0.1^{h} 0.009^{h}	0.1^{h} 0.009^{h}	0.1^{f} 0.01^{d}	0.1^{f} 0.01^{d}	0.1^{f} 0.01^{d}
U (red.) U (ox.)	5^{a} 0.1^{d} 1^{c} 0.01^{d}	5^{a} 0.1^{d} 1^{c} 0.01^{d}	1^{a} 0.1^{d} 0.1^{c} 0.01^{d}	5^{a} 0.1^{d} 1^{c} 0.01^{d}	5^{a} 0.1^{d} 1^{c} 0.01^{d}	1^{a} 0.1^{d} 0.1^{c} 0.01^{d}	1^{g} 0.01^{g}	1^{g} 0.01^{g}	1^{g} 0.01^{g}	1^{h} 0.01^{h}	1^{h} 0.01^{h}	1^{h} 0.01^{h}	1^{f} 0.01^{d} 0.02^{f} 0.001^{d}	1^{f} 0.01^{d} 0.02^{f} 0.001^{d}	1^{f} 0.01^{d} 0.02^{f} 0.001^{d}
Np (red.) Np (ox.)	5^{a} 0.1^{d} 2^{c} 0.01^{d}	5^{a} 0.1^{d} 2^{c} 0.01^{d}	1^{a} 0.1^{d} 0.2^{c} 0.01^{d}	5^{a} 0.1^{d} 2^{c} 0.01^{d}	5^{a} 0.1^{d} 2^{c} 0.01^{d}	1^{a} 0.1^{d} 0.2^{c} 0.01^{d}	3^{g} 0.1^{g}	3^{g} 0.1^{g}	3^{g} 0.1^{g}	1^{h} 0.02^{h}	1^{h} 0.02^{h}	1^{h} 0.02^{h}	1^{f} 0.01^{d} 0.02^{f} 0.001^{d}	1^{f} 0.01^{d} 0.02^{f} 0.001^{d}	1^{f} 0.01^{d} 0.02^{f} 0.001^{d}
Am	0.25^{q} 0.0025^{p}	0.25^{q} 0.0025^{p}	0.05^{q} 0.0025^{p}	5^{a} 0.0025^{p}	5^{a} 0.0025^{p}	1^{a} 0.0025^{p}	3^{g} 0.05^{r}	3^{g} 0.05^{r}	3^{g} 0.05^{r}	1^{h} 0.005^{h}	1^{h} 0.005^{h}	1^{h} 0.005^{h}	1^{f} $5E\text{-}04^{v}$	1^{f} $5E\text{-}04^{v}$	1^{f} $5E\text{-}04^{v}$
Cm	0.25^{q} 0.0025^{p}	0.25^{q} 0.0025^{p}	0.05^{q} 0.0025^{p}	5^{a} 0.0025^{p}	5^{a} 0.0025^{p}	1^{a} 0.0025^{p}	3^{g} 0.05^{r}	3^{g} 0.05^{r}	3^{g} 0.05^{r}	1^{h} 0.005^{h}	1^{h} 0.005^{h}	1^{h} 0.005^{h}	1^{f} $5E\text{-}04^{v}$	1^{f} $5E\text{-}04^{v}$	1^{f} $5E\text{-}04^{v}$

[a] Table 2.4, Savage et al. (2000); [b] Table 4, Bradbury and Sarott (1995); [c] Table 5.1, Krupka and Serne (1999); [d] arbitrary value for sensitivity analysis; [e] Table 9-3, Vieno and Nordman (1998); [f] Stenhouse (1995); [g] Table A2.3.2, Anderson (1999); [h] = $0.9 \cdot K_d$ (sand) + $0.1 \cdot K_d$ (compacted bentonite); [m]: Effect of organics: sorption reduction factors for Pu (Table 5) and for certain other elements relative to Pu (Table 9), Bradbury and Sarott (1995); [p]: = e + m; [q]: = a + m; [r]: = g + m; [v]: = d + m.

Table 3.1 (continued) Best estimate and pessimistic K_d values for sorption on different substrates (m^3/kg).

	Best Estimate and Pessimistic K_d Values (m^3/kg)		
	Waste matrix [BMA] *(porous concrete)*		
	I	***II***	***III***
Pu	0.01 [q] 2E-04 [v]	0.01 [q] 2E-04 [v]	0.002 [q] 2E-04 [v]
Ra	0.05 [a] 0.005 [d]	0.05 [a] 0.005 [d]	0.05 [a] 0.005 [d]
Ac [=Am]	0.01 1E-04	0.01 1E-04	0.002 1E-04
Th	0.01 [q] 2E-04 [v]	0.01 [q] 2E-04 [v]	0.002 [q] 2E-04 [v]
Pa	0.2 [q] 0.04 [v]	0.2 [q] 0.04 [v]	0.04 [q] 0.004 [v]
U (red.) U (ox.)	2 [q] 0.04 [v] 0.4 [w] 0.004 [v]	2 [q] 0.04 [v] 0.4 [w] 0.004 [v]	0.4 [q] 0.04 [v] 0.04 [w] 0.004 [v]
Np (red.) Np (ox.)	2 [q] 0.04 [v] 0.8 [w] 0.004 [v]	2 [q] 0.04 [v] 0.8 [w] 0.004 [v]	0.4 [q] 0.04 [v] 0.08 [w] 0.004 [v]
Am	0.01 [q] 1E-04 [p]	0.01 [q] 1E-04 [p]	0.002 [q] 1E-04 [p]
Cm	0.01 [q] 1E-04 [p]	0.01 [q] 1E-04 [p]	0.002 [q] 1E-04 [p]

[a] Table 2.4, Savage et al. (2000); [d] arbitrary value for sensitivity analysis; [e] Table 9-3, Vieno and Nordman (1998);
[m]: Effect of organics: sorption reduction factors for Pu (Table 5) and for certain other elements relative to Pu (Table 9), Bradbury and Sarott (1995); [p]: = e + m; [q]: = a + m; [v]: = d + m; [w]:= c + m.

Table 3.1 (continued) Best estimate and pessimistic K_d values for sorption on different substrates (m^3/kg): saline conditions.

	Best Estimate and Pessimistic K_d Values (m^3/kg)														
	Backfill (crushed rock)			*Near-field rock: fractures*			*Near-field rock: matrix*			*Far-field rock: fractures*			*Far-field rock: matrix*		
	I	***II***	***III***	***I***	***II***	***III***	***I***	***II***	***III***	***I***	***II***	***III***	***I***	***II***	***III***
C	0.001^{g} 0^{d}	0.001^{g} 0^{d}	0.001^{g} 0^{d}	0.001^{o} 0^{o}	0.001^{o} 0^{o}	0.001^{o} 0^{o}	0.001^{g} 0^{d}	0.001^{g} 0^{d}	0.001^{g} 0^{d}	0.001^{o} 0^{o}	0.001^{o} 0^{o}	0.001^{o} 0^{o}	0.001^{g} 0^{d}	0.001^{g} 0^{d}	0.001^{g} 0^{d}
Fe [=Ni]	0.02 0.005	0.02 0.005	0.02 0.005	0.5 0.005	0.5 0.005	0.5 0.005	0.02 0.005	0.02 0.005	0.02 0.005	0.5 0.005	0.5 0.005	0.5 0.005	0.02 0.005	0.02 0.005	0.02 0.005
Ni	0.02^{k} 0.005^{d}	0.02^{k} 0.005^{d}	0.02^{k} 0.005^{d}	0.5^{o} 0.005^{d}	0.5^{o} 0.005^{d}	0.5^{o} 0.005^{d}	0.02^{k} 0.005^{d}	0.02^{k} 0.005^{d}	0.02^{k} 0.005^{d}	0.5^{o} 0.005^{d}	0.5^{o} 0.005^{d}	0.5^{o} 0.005^{d}	0.02^{k} 0.005^{d}	0.02^{k} 0.005^{d}	0.02^{k} 0.005^{d}
Co [=Ni]	0.02 0.005	0.02 0.005	0.02 0.005	0.5 0.005	0.5 0.005	0.5 0.005	0.02 0.005	0.02 0.005	0.02 0.005	0.5 0.005	0.5 0.005	0.5 0.005	0.02 0.005	0.02 0.005	0.02 0.005
Sr ($x10^5$)	2^{i} 1^{i}	2^{i} 1^{i}	2^{i} 1^{i}	500^{f} 1^{d}	500^{f} 1^{d}	500^{f} 1^{d}	2^{i} 1^{i}	2^{i} 1^{i}	2^{i} 1^{i}	500^{f} 1^{d}	500^{f} 1^{d}	500^{f} 1^{d}	2^{i} 1^{i}	2^{i} 1^{i}	2^{i} 1^{i}
Nb	1^{k} 0.1^{d}	1^{k} 0.1^{d}	1^{k} 0.1^{d}	1^{o} 0.1^{o}	1^{o} 0.1^{o}	1^{o} 0.1^{o}	1^{k} 0.1^{d}	1^{k} 0.1^{d}	1^{k} 0.1^{d}	1^{o} 0.1^{o}	1^{o} 0.1^{o}	1^{o} 0.1^{o}	1^{k} 0.1^{d}	1^{k} 0.1^{d}	1^{k} 0.1^{d}
Tc (red.) Tc (ox.)	1^{k} 0.1^{d} 0^{k} ---	1^{k} 0.1^{d} 0^{k} ---	1^{k} 0.1^{d} 0^{k} ---	0.5^{o} 0.05^{o} 0^{k} ---	0.5^{o} 0.05^{o} 0^{k} ---	0.5^{o} 0.05^{o} 0^{k} ---	1^{k} 0.1^{d} 0^{k} ---	1^{k} 0.1^{d} 0^{k} ---	1^{k} 0.1^{d} 0^{k} ---	0.5^{o} 0.05^{o} 0^{k} ---	0.5^{o} 0.05^{o} 0^{k} ---	0.5^{o} 0.05^{o} 0^{k} ---	1^{k} 0.1^{d} 0^{k} ---	1^{k} 0.1^{d} 0^{k} ---	1^{k} 0.1^{d} 0^{k} ---
Ru [=Pd]	0.01^{k} 0.001^{k}	0.01^{k} 0.001^{k}	0.01^{k} 0.001^{k}	0.5^{o} 0.001^{d}	0.5^{o} 0.001^{d}	0.5^{o} 0.001^{d}	0.01^{k} 0.001^{k}	0.01^{k} 0.001^{k}	0.01^{k} 0.001^{k}	0.5^{o} 0.001^{d}	0.5^{o} 0.001^{d}	0.5^{o} 0.001^{d}	0.01^{k} 0.001^{k}	0.01^{k} 0.001^{k}	0.01^{k} 0.001^{k}
I	0^{k} ---	0^{k} ---	0^{k} ---	0.0005^{l} 0^{o}	0.0005^{l} 0^{o}	0.0005^{l} 0^{o}	0^{k} ---	0^{k} ---	0^{k} ---	0.0005^{l} 0^{o}	0.0005^{l} 0^{o}	0.0005^{l} 0^{o}	0^{k} ---	0^{k} ---	0^{k} ---
Cs	0.05^{k} 0.01^{k}	0.05^{k} 0.01^{k}	0.05^{k} 0.01^{k}	0.1^{o} 0.01^{o}	0.1^{o} 0.01^{o}	0.1^{o} 0.01^{o}	0.05^{k} 0.01^{k}	0.05^{k} 0.01^{k}	0.05^{k} 0.01^{k}	0.1^{o} 0.01^{o}	0.1^{o} 0.01^{o}	0.1^{o} 0.01^{o}	0.05^{k} 0.01^{k}	0.05^{k} 0.01^{k}	0.05^{k} 0.01^{k}
Pb	1^{j} 0.05^{d}	1^{j} 0.05^{d}	1^{j} 0.05^{d}	0.5^{o} 0.05^{o}	0.5^{o} 0.05^{o}	0.5^{o} 0.05^{o}	1^{j} 0.05^{d}	1^{j} 0.05^{d}	1^{j} 0.05^{d}	0.5^{o} 0.05^{o}	0.5^{o} 0.05^{o}	0.5^{o} 0.05^{o}	1^{j} 0.05^{d}	1^{j} 0.05^{d}	1^{j} 0.05^{d}
Po [=Pb]	1 0.05	1 0.05	1 0 05	0.5 0.05	0.5 0.05	0.5 0.05	1 0.05	1 0.05	1 0.05	0.5 0.05	0.5 0.05	0.5 0.05	1 0.05	1 0.05	1 0.05

[a] Table 2.4, Savage et al. (2000); [b] Table 4, Bradbury and Sarott (1995); [c] Table 5.1, Krupka and Serne (1999); [d] arbitrary value for sensitivity analysis;[e] Table 9-3, Vieno and Nordman (1998); [f] Appendix B, Stenhouse (1995); [i]: Bruno and Duro (1997); [j]: Albinsson (1991); [k] Table 12-1, Carbol and Engkvist (1997) - also Table A2.6.2, Andersson (1999); [l]:Andersson (1996); [m]: Effect of organics: sorption reduction factors for Pu (Table5) and for certain other elements relative to Pu (Table 9), Bradbury and Sarott (1995); [o]: Table 10, Stenhouse (1995).

Table 3.1 (continued) Best estimate and pessimistic K_d values for sorption on different substrates (m^3/kg).

	Best Estimate and Pessimistic K_d Values (m^3/kg)														
	Backfill (crushed rock)			*Near-field rock: fractures*			*Near-field rock: matrix*			*Far-field rock: fractures*			*Far-field rock: matrix*		
	I	***II***	***III***	***I***	***II***	***III***	***I***	***II***	***III***	***I***	***II***	***III***	***I***	***II***	***III***
Pu	5^{k} 0.005^{v}	5^{k} 0.005^{v}	5^{k} 0.005^{v}	5^{o} 0.005^{v}	5^{o} 0.005^{v}	5^{o} 0.005^{v}	5^{k} 0.005^{v}	5^{k} 0.005^{v}	5^{k} 0.005^{v}	5^{o} 0.005^{v}	5^{o} 0.005^{v}	5^{o} 0.005^{v}	5^{k} 0.005^{v}	5^{k} 0.005^{v}	5^{k} 0.005^{v}
Ra	0.02^{g} 0.005^{d}	0.02^{g} 0.005^{d}	0.02^{g} 0.005^{d}	0.2^{o} 0.005^{d}	0.2^{o} 0.005^{d}	0.2^{o} 0.005^{d}	0.02^{g} 0.005^{d}	0.02^{g} 0.005^{d}	0.02^{g} 0.005^{d}	0.2^{o} 0.005^{d}	0.2^{o} 0.005^{d}	0.2^{o} 0.005^{d}	0.02^{g} 0.005^{d}	0.02^{g} 0.005^{d}	0.02^{g} 0.005^{d}
Ac [=Am]	3^{k} 0.005^{v}	3^{k} 0.005^{v}	3^{k} 0.005^{v}	5^{o} 0.005^{v}	5^{o} 0.005^{v}	5^{o} 0.005^{v}	3^{k} 0.005^{v}	3^{k} 0.005^{v}	3^{k} 0.005^{v}	5^{o} 0.005^{v}	5^{o} 0.005^{v}	5^{o} 0.005^{v}	3^{k} 0.005^{v}	3^{k} 0.005^{v}	3^{k} 0.005^{v}
Th	5^{k} 0.005^{v}	5^{k} 0.005^{v}	5^{k} 0.005^{v}	1^{o} 0.005^{u}	1^{o} 0.005^{u}	1^{o} 0.005^{u}	5^{k} 0.005^{v}	5^{k} 0.005^{v}	5^{k} 0.005^{v}	1^{o} 0.005^{u}	1^{o} 0.005^{u}	1^{o} 0.005^{u}	5^{k} 0.005^{v}	5^{k} 0.005^{v}	5^{k} 0.005^{v}
Pa	1^{k} 0.1^{d}	1^{k} 0.1^{d}	1^{k} 0.1^{d}	1^{o} 0.1^{o}	1^{o} 0.1^{o}	1^{o} 0.1^{o}	1^{k} 0.1^{d}	1^{k} 0.1^{d}	1^{k} 0.1^{d}	1^{o} 0.1^{o}	1^{o} 0.1^{o}	1^{o} 0.1^{o}	1^{k} 0.1^{d}	1^{k} 0.1^{d}	1^{k} 0.1^{d}
U (red.) U (ox.)	5^{k} 0.1^{d} 0.005^{k} 0.001^{k}	5^{k} 0.1^{d} 0.005^{k} 0.001^{k}	5^{k} 0.1^{d} 0.005^{k} 0.001^{k}	1^{o} 0.1^{o} 0.005^{k} 0.001^{k}	1^{o} 0.1^{o} 0.005^{k} 0.001^{k}	1^{o} 0.1^{o} 0.005^{k} 0.001^{k}	5^{k} 0.1^{d} 0.005^{k} 0.001^{k}	5^{k} 0.1^{d} 0.005^{k} 0.001^{k}	5^{k} 0.1^{d} 0.005^{k} 0.001^{k}	1^{o} 0.1^{o} 0.005^{k} 0.001^{k}	1^{o} 0.1^{o} 0.005^{k} 0.001^{k}	1^{o} 0.1^{o} 0.005^{k} 0.001^{k}	5^{k} 0.1^{d} 0.005^{k} 0.001^{k}	5^{k} 0.1^{d} 0.005^{k} 0.001^{k}	5^{k} 0.1^{d} 0.005^{k} 0.001^{k}
Np (red.) Np (ox.)	5^{k} 0.1^{d} 0.005^{k} 0.001^{k}	5^{k} 0.1^{d} 0.005^{k} 0.001^{k}	5^{k} 0.1^{d} 0.005^{k} 0.001^{k}	1^{o} 0.1^{o} 0.005^{k} 0.001^{k}	1^{o} 0.1^{o} 0.005^{k} 0.001^{k}	1^{o} 0.1^{o} 0.005^{k} 0.001^{k}	5^{k} 0.1^{d} 0.005^{k} 0.001^{k}	5^{k} 0.1^{d} 0.005^{k} 0.001^{k}	5^{k} 0.1^{d} 0.005^{k} 0.001^{k}	1^{o} 0.1^{o} 0.005^{k} 0.001^{k}	1^{o} 0.1^{o} 0.005^{k} 0.001^{k}	1^{o} 0.1^{o} 0.005^{k} 0.001^{k}	5^{k} 0.1^{d} 0.005^{k} 0.001^{k}	5^{k} 0.1^{d} 0.005^{k} 0.001^{k}	5^{k} 0.1^{d} 0.005^{k} 0.001^{k}
Am	3^{k} 0.005^{v}	3^{k} 0.005^{v}	3^{k} 0.005^{v}	5^{o} 0.005^{v}	5^{o} 0.005^{v}	5^{o} 0.005^{v}	3^{k} 0.005^{v}	3^{k} 0.005^{v}	3^{k} 0.005^{v}	5^{o} 0.005^{v}	5^{o} 0.005^{v}	5^{o} 0.005^{v}	3^{k} 0.005^{v}	3^{k} 0.005^{v}	3^{k} 0.005^{v}
Cm	3^{k} 0.005^{v}	3^{k} 0.005^{v}	3^{k} 0.005^{v}	5^{o} 0.005^{v}	5^{o} 0.005^{v}	5^{o} 0.005^{v}	3^{k} 0.005^{v}	3^{k} 0.005^{v}	3^{k} 0.005^{v}	5^{o} 0.005^{v}	5^{o} 0.005^{v}	5^{o} 0.005^{v}	3^{k} 0.005^{v}	3^{k} 0.005^{v}	3^{k} 0.005^{v}

[a] Savage et al. (2000); [b]: Table 4, Bradbury and Sarott (1995); [c] Table 5.1, Krupka and Serne (1999); [d] arbitrary value for sensitivity analysis;
[e] Table 9-3, Vieno and Nordman (1998); (1998); [f] Appendix B, Stenhouse (1995); [g] Tables A.2.3.2 (compacted bentonite) and A.2.6.2 (granitic rock), Anderson (1999);
[h] Table 10, Stenhouse (1995); [i]: Bruno and Duro (1997); [j]: Albinsson (1991); [k] Table 12-1, Carbol and Engkvist (1997); [l] Andersson (1996); [m]: Effect of organics: sorption reduction factors for Pu (Table 5) and for certain other elements relative to Pu (Table 9), Bradbury and Sarott (1995); [o]: Table 10, Stenhouse (1995);
[r]: = g + m; [s]: = k + m; [u]: = o + m; [v]: = d + m.

4 Solubility data

Although radionuclide release in groundwater at SFR 1 is unlikely to be limited by elemental solubility limits, solubility data have been assembled as reference data. These data were taken without critical review from a recent compilation of data for the disposal of long-lived intermediate-level radioactive waste in Japan (JNC, 2000). These data include variation of solubility with pH with time according to the evolution of cement chemistry defined here in Section 1. However for the most part, these data are insensitive to pH variations (Sr, Nb, Tc, I, Cs, Pb, Po, Pu, Ra, Pa, U).

Table 4.1 Solubility data for radionuclides (mol/L). Data from JNC (2000).

	I	**II**	**III**
C	7E-08	7E-05	1E-05
Fe [=Ni]	2E-04	3E-05	2E-06
Ni	2E-04	3E-05	2E-06
Co	2E-04	3E-05	2E-06
Sr	1E-04	1E-04	1E-04
Nb	soluble	soluble	soluble
Tc (red.)	4E-08	4E-08	4E-08
Ru [=Pd]	3E-07	3E-08	7E-09
I	soluble	soluble	soluble
Cs	soluble	soluble	soluble
Pb	soluble	soluble	soluble
Po [=Pb]	soluble	soluble	soluble
Pu	1E-10	1E-10	1E-10
Ra	1E-06	1E-06	1E-06
Ac	3E-09	4E-09	4E-09
Th	6E-10	7E-10	8E-10
Pa	2E-08	2E-08	2E-08
U (red.)	1E-08	1E-08	1E-08
Np (red.)	5E-09	5E-09	6E-09
Am	2E-09	3E-09	9E-09
Cm	2E-09	3E-09	9E-09

5 Gas issues

5.1 Factors affecting gas generation rates

From a performance assessment (PA) perspective, the key questions to be addressed when dealing with the topic of gas in a radioactive waste repository are:

- will gas be produced in the repository?

If so,

- under what conditions will gas be generated?
- how much gas will be produced?
- at what rate will the gas be produced?
- what are the potential impacts from any gas generated?

The above questions are discussed below.

5.1.1 Will gas be produced?

Given the typical inventory of materials (waste, structural components) in a radioactive waste repository, gas (H_2) will be generated from the corrosion of substantial quantities of metals, principally steel and aluminium, and to a lesser extent, zirconium (zircalloy), present in the waste itself. Corrosion of steel present in the reinforced concrete structures (e.g. Silo of SFR 1) will also occur. Additional gas (CO_2, CH_4) will be generated from the degradation of any organic material present - cellulose and other organics such as ion exchange resins, bitumen and plastics. Radiolytic decomposition of water can also lead to H_2 generation but can be neglected for the SFR 1 repository owing to the relatively low radiation levels expected.

5.1.2 Under what conditions will gas be generated?

Moisture is necessary for the corrosion of metals. In addition, anaerobic conditions will result in the production of H_2 from the corrosion of steel (Fe). Alkaline conditions (i.e. high pH) promote the dissolution of the outer (passivating) oxide coating on aluminium, thereby exposing fresh surface and accelerating the corrosion of this metal. In the case of zircalloy, the outer oxide coating is not dissolved under alkaline conditions and the corresponding corrosion rate is slow.

For the degradation of organic material, moisture and the availability of microbes are necessary. Although microbial degradation favours less alkaline conditions than those likely to exist in a cementitious repository, such degradation cannot be discounted and is generally assumed to occur.

5.1.3 How much gas will be generated?

This question depends directly on the inventory (quantity) and surface area of those materials which degrade to produce gas, *i.e.* steel, aluminium, (zirconium as a significant source of H_2 can effectively be ignored owing to its low corrosion rate and relatively low quantity of the waste inventory), cellulose and other organics. Besides the waste itself, the quantity of steel present in reinforced structures must be known, since the corrosion of such structural materials will generate additional H_2. Stoichiometric equations can be written to describe the corrosion of metals and the degradation of organics. In the latter case, the gases produced are CO_2 and CH_4, the proportion of each being variable and depending on what reaction sequence actually occurs; the latter depends, in turn, on the amount of oxidants (O_2, nitrate, sulphate or carbonate) available. Microbial activity requires access to certain nutrients at trace levels, including phosphorus and certain trace metals.

5.1.4 At what rate will gases be generated?

Gas generation rates will depend on corrosion rates and surface areas of the corresponding metals undergoing corrosion. Some uncertainty exists regarding the rates of corrosion/degradation of different materials under repository conditions, which should, therefore, be reflected in a possible range of (bounding) corrosion rates for each type of material considered. Typical rates quoted elsewhere for the two important metals agree with those cited in Skagius et al. (1999); i.e. cited in Lindgren and Pers (1994), viz.

- Steel: 1 µm/y quoted by Agg et al. (1993) and Grogan et al. (1992); relevant Japanese experimental data indicate a corrosion rate < 0.1 µm/y (Impey et al., 1995);
- Aluminium: 1 mm/y quoted by Agg et al. (1993) and Grogan et al. (1992); relevant Japanese experimental data indicate ~ 0.1 mm/year (Impey et al., 1995).

5.1.5 What are the impacts from gases generated in the repository?

The potential impacts from any gas generated concern:

- a radiological hazard from the transport of radioactive gases to the biosphere;
- a flammability hazard from gases transported to the biosphere;
- the potential consequences of a build-up in gas pressure within one or more of the repository barriers, i.e.
    - disruption of barriers, influencing the groundwater pathway, and/or

- displacement of water, possibly contaminated, from the repository zone; hence, faster radionuclide transport via the groundwater pathway.

Radiological hazard

Radioactive gases normally considered in safety assessments are $^3H_2$ (tritiated hydrogen), $^{14}CO_2$, $^{14}CH_4$, ^{129}I and radon gases. Conservative assumptions may be made about the fraction of the inventory of these radionuclides which can be incorporated as a gas. For the most conservative treatment, some safety assessments "double-count" the tritium and ^{14}C inventories for the purpose of radionuclide transport and associated dose calculations via the gas and groundwater exposure pathways (e.g. Kozak et al., 2000), i.e. assume the entire inventory of each radionuclide (^3H and ^{14}C) is available for both pathways. Clearly, this is unrealistic for the situation where a significant component of the waste inventory includes, for example, ^{14}C in activated metal.

Flammability hazard

Hydrogen and/or methane both constitute a flammability/explosive hazard if either gas is present in an enclosed volume at significant concentration (in air): 4–74% for H_2 and 5–15% for CH_4 (Lewis and von Elbe, 1951). Thus, the possibility should be considered of some conduit (focussed pathway such as a fault or fracture zone) from the repository directly to the surface and subsequent release into a dwelling/building. Given the depth of the SFR 1 repository, the likelihood of a focussed release over several hundred metres is small.

Build-up in gas pressure

Gas generation will result in the gradual formation of a gas phase and some build-up of gas pressure, the nature and extent of this pressure being dependent on a number of factors:

- connectivity between waste packages and other barriers of the near field;
- amount of void space in different parts of the repository (waste package, grout, concrete shell, backfill, near-field rock);
- ability of gas to move through, and between, individual barriers, thereby dissipating excess pressure.

The latter requires that the water present in (at least some of) the pores of a saturated medium must be displaced which depends in turn on the capillary forces of the material concerned, i.e. porous cement, concrete or bentonite or sand-bentonite.

Possible impacts, depending on the extent of gas pressure build-up, include:

- displacement of water from different barriers; depending on when this happens, such an impact may be;
  - advantageous, by restricting water access to degrading materials, thereby reducing the rate of gas generation; or
  - detrimental if, following canister failure, the water displaced is contaminated with radionuclides.
- disruption of near-field barriers, thereby potentially affecting radionuclide release and transport by creating faster pathways, e.g. irreversible displacement of bentonite backfill, creating preferential pathways for radionuclide (advective) transport in groundwater.

Given significant quantities of CO_2 produced from the degradation of organic material, reaction of dissolved CO_2 with resultant precipitation of $CaCO_3$ can occur which will reduce (even clog) available porosity and may, in turn, influence available gas pathways.

The essential factors of the above topics and information are represented as features, events and processes (FEPs) and interactions between FEPs (Influences) in *Figure 5.1*, a portion of an Influence Diagram focussing on gas issues, applicable to the Silo section of the SFR 1 repository (this would also apply to the SFL-3 repository), which has the greatest number of engineered barriers. Moving from the left side to the right side of this diagram corresponds to the different barriers of the near field: waste package, cement grout/mortar, concrete (steel reinforced) shell, backfill (bentonite, sand-bentonite) and near-field rock.

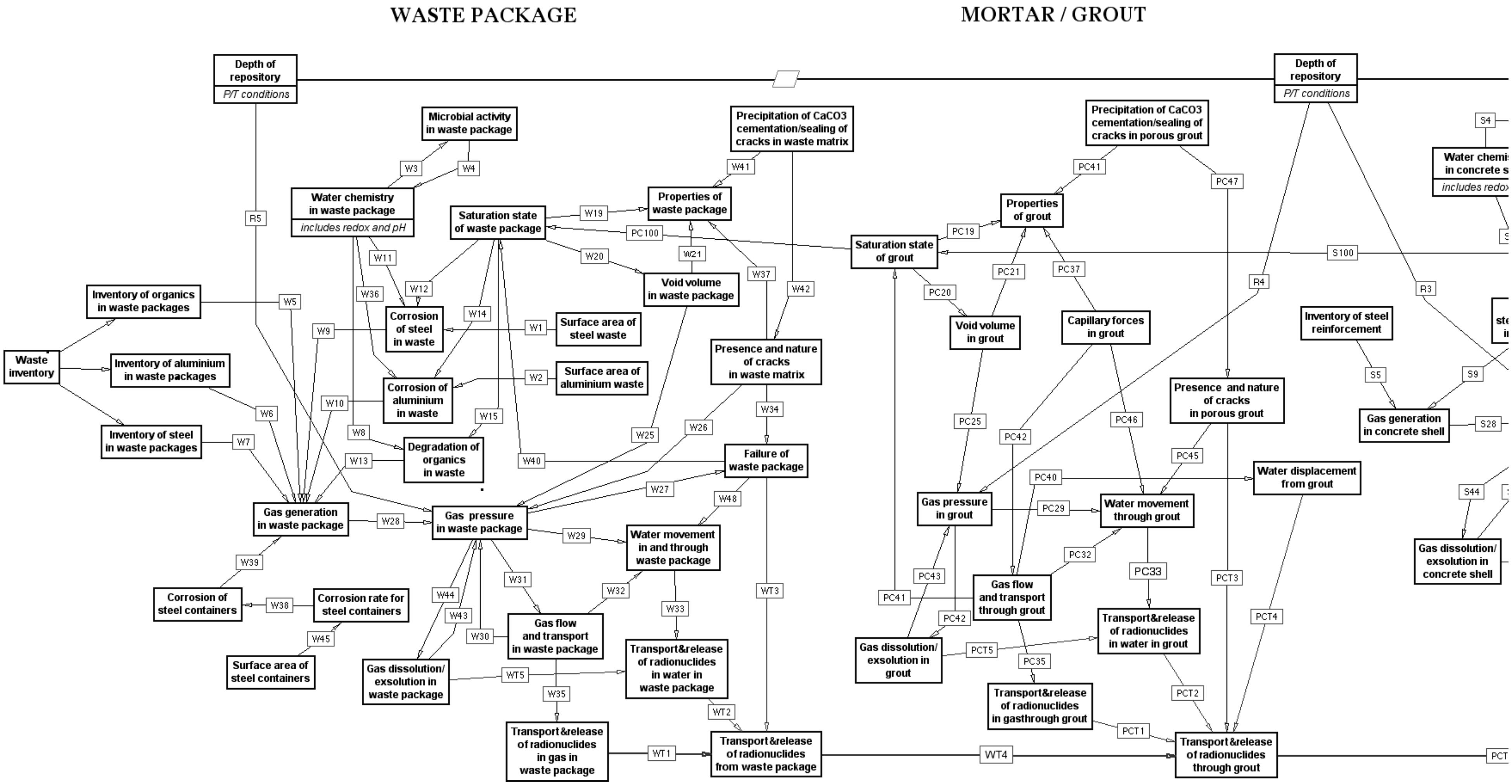

Figure 5.1 Features, Events and Processes (FEPs) and Influences related to gas generation and impacts in a radioactive waste repository.

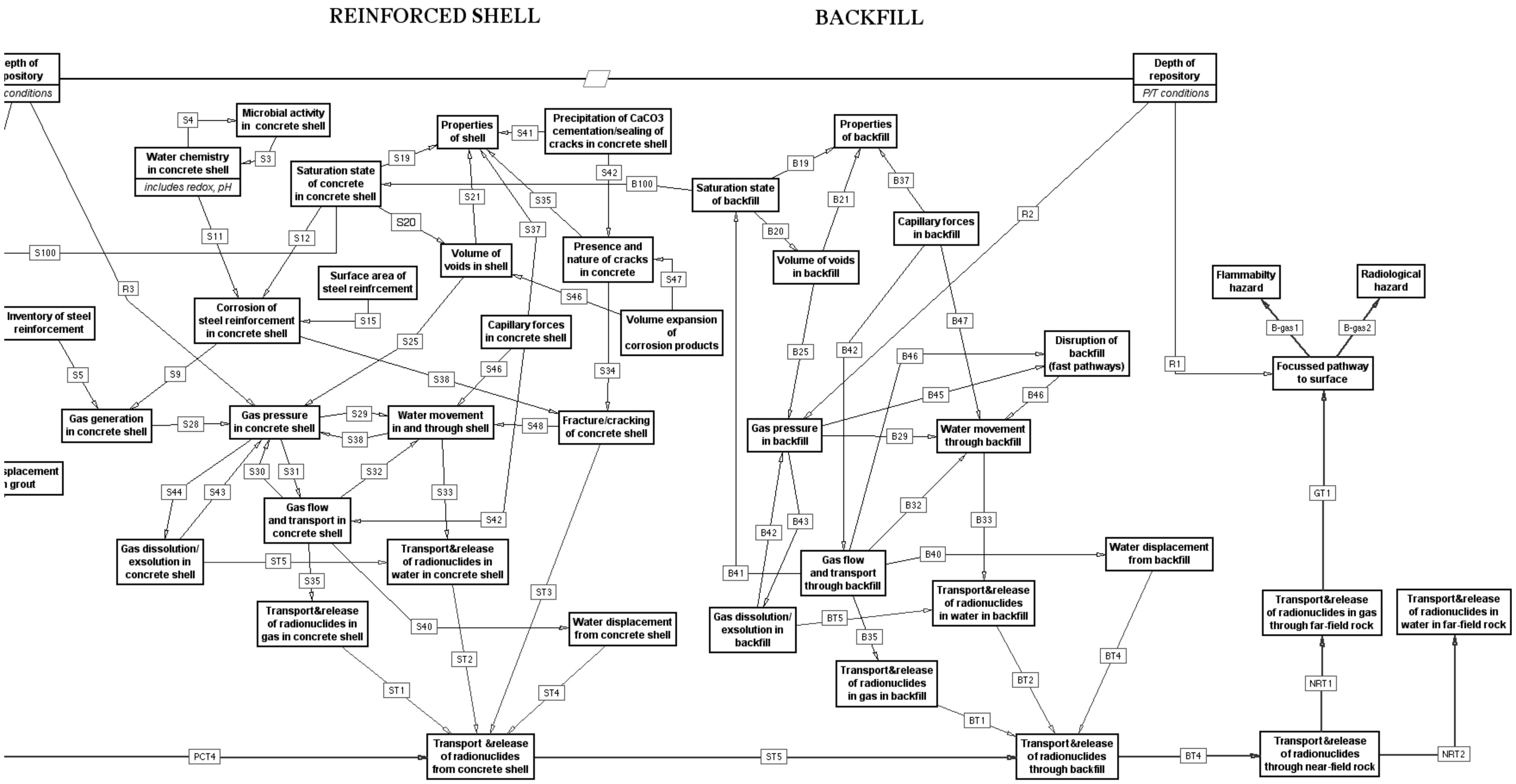

Figure 5.1 (continued) Features, Events and Processes (FEPs) and Influences related to gas generation and impacts in a radioactive waste repository.

5.2 Review of "Gas generation in SFL 3-5 and effects on radionuclide release" (Skagius et al., 1999)

The above report was reviewed in the context of its relevance to the SFR 1 repository and most of the comments/queries provided below are, therefore, general in nature. Issues relating to quantities and rates of gas production, and volume of voids available, are repository-specific, and depend on inventories of repository materials. However, similar issues concerning calculation of these quantities are likely to arise for the SFR 1 repository.

5.2.1 Comments/Queries - General

The topics discussed in Section 5.1 of this report are addressed in detail in Skagius et al., (1999). With respect to Section 5.1.5 (impacts of gas generated), there is no discussion of radiological impacts or flammability hazards. These can be suitably addressed via relatively simple scoping calculations (see, for example, Kozak et al., 2000).

For the calculations, each component of the SFL 3-5 repository is considered separately, implying no connectivity between individual components. This situation may not apply to the SFR 1 repository where, the different components (silo, vaults, tunnel) are located much closer.

In the calculations, a fully re-saturated repository is assumed [*p. 41, par. 4*] which seems reasonable. Also, in Section 5, the amount of water required for corrosion is specified as a percentage of full saturation, implying that the corrosion rate would be less if less water were available. The question arises whether there are any circumstances under which a slower build-up in gas would be more detrimental (than a faster rate)? A reduced corrosion rate could happen if, for example, an overpressure within a waste package prevents water from reaching the waste. The only concern in this context appears to be that, with more time elapsed, the likelihood of an "on-site" dwelling increases. However, under the same circumstances, the likelihood of a focussed pathway for gas from the repository to the surface probably decreases. Thus, the assumption of a fully-resaturated repository appears conservative.

One of the major conclusions from the gas study is that significant overpressures are predicted such that cracking will occur in the concrete and backfill barriers, enough to allow gas to escape without major disruption of barriers. This implies that the hydraulic properties of these barriers could be increased significantly enough to affect the transport parameter values for the groundwater pathway.

The gas and groundwater pathways are typically tackled separately in assessment calculations, but there needs to be some link between the two to take into account any impacts that a build-up in gas pressure might have on the groundwater pathway (e.g. increased hydraulic conductivities of one or more barriers).

The study predicts that large volumes (relative to available void space) of H_2 will be generated in the first few years due to corrosion of aluminium. Since the concrete barrier presumably is expected to be intact during this period, i.e. capillary pressure of 1 to 2 MPa, there is a need to examine this early period for evidence of conservative assumptions (e.g. corrosion rate of aluminium), particularly when there are safety aspects concerning the operational phase.

Given the production of CO_2 from the microbial degradation of organic materials, the clogging of pores due to precipitation of $CaCO_3$ (carbonation) could provide a mechanism for sealing small fractures/cracks, reducing the gas permeability of the concrete barrier, and thereby increasing the potential for even greater gas pressure build-up with a subsequently much larger fracture/crack or even failure of the barrier.

Similarly, the formation of corrosion products and the resultant expansion in volume will reduce the void space available for gas. The possible impact of this effect is considered negligible in the report [*p. 41, last par.* "*Volume expansion of corrosion products probably gives negligible effect, possibly cracking around reinforcement causing weaknesses but no fully penetrating fractures or cracks.*"]

5.2.2 Comments/Queries – More Specific

With respect to corrosion rates for steel, aluminium and zircalloy [*p. 15*], although the values quoted in the report appear to be conservative compared with others quoted elsewhere (see Section 5.1), it should be noted that Wiborgh (1995) previously cited a corrosion rate for Al in the range 1-10 mm/y and a corrosion rate for Fe in the range 0.1-10 µm/y (Höglund and Bengtsson, 1991). In this respect, the values of corrosion rate used in the calculations are not bounding. The influence of groundwater chemistry, (e.g. Cl^-) on an increased corrosion rate of steel does not appear to have been considered explicitly. For a given inventory, the rates of corrosion affect directly the timescale over which gas is generated and, hence, the nature and time dependency of possible impacts of the gases produced (next question).

The report states [p. 21, last sentence] that an increase in gas pressure inside the bentonite barrier would occur during the first 5 years "if the void accessible to gas in waste packages, porous concrete and concrete structures is around 40% of the total void" volume. If the bentonite is not fully saturated in this time period, gas flow could disrupt this barrier.

Figure 5-7 [p. 27] indicates that *"capillary pressure will determine the internal overpressure required for gas escape as long as the fractures are wider than 0.07 mm…….and i*S >1…….for these combinations of fractures geometry, an internal overpressure of about 2 to 3 kPa is enough to allow gas escape through the concrete lid."* The conclusion is that the intact concrete will degrade to a state where the calculational basis is reasonable. However, this may not be relevant to the first few years, when concrete remains intact and gas production from the corrosion of aluminium is great.

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