Project SAFE

Compilation of data for radionuclide transport analysis

Svensk Kärnbränslehantering AB

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Abstract

This report is one of the supporting documents to the updated safety assessment (project SAFE) of the Swedish repository for low and intermediate level waste, SFR 1. A number of calculation cases for quantitative analysis of radionuclide release and dose to man are defined based on the expected evolution of the repository, geosphere and biosphere in the Base Scenario and other scenarios selected. The data required by the selected near field, geosphere and biosphere models are given and the values selected for the calculations are compiled in tables. The main sources for the selected values of the migration parameters in the repository and geosphere models are the safety assessment of a deep repository for spent fuel, SR 97, and the preliminary safety assessment of a repository for long-lived, low- and intermediate level waste, SFL 3-5. For the biosphere models, both site-specific data and generic values of the parameters are selected.

The applicability of the selected parameter values is discussed and the uncertainty is qualitatively addressed for data to the repository and geosphere migration models. Parameter values selected for these models are in general pessimistic in order not to underestimate the radionuclide release rates. It is judged that this approach combined with the selected calculation cases will illustrate the effects of uncertainties in processes and events that affects the evolution of the system as well as in quantitative data that describes this. The biosphere model allows for probabilistic calculations and the uncertainty in input data are quantified by giving minimum, maximum and mean values as well as the type of probability distribution function.

Sammanfattning

Denna rapport utgör ett av stöddokumenten till den uppdaterade säkerhetsanalysen (projekt SAFE) av SFR 1, det svenska förvaret för låg- och medelaktivt avfall. Ett antal beräkningsfall för kvantitativ analys av radionuklidutsläpp och resulterande dos till människa definieras utgående från den förväntade utvecklingen av förvarets, geosfärens och biosfärens tillstånd för Basscenariot och övriga valda scenarier. De indata som behövs till de valda förvars-, geosfärs- och biosfärsmodellerna redovisas och de värden som valts sammanställs i tabeller. Värden på migrationsparametrarna i förvars- och geosfärsmodellen har huvudsakligen valts från den nyligen genomförda säkerhets-analysen av ett djupförvar för utbränt kärnbränsle, SR 97, och från den preliminära säkerhetsanalysen av ett förvar för långlivat, låg- och medelaktivt avfall, SFL 3-5. Som indata till biosfärsmodellen har både platsspecifika värden och generiska värden valts.

Tillämpligheten av de värden som valts för parametrarna i förvars- och geosfärs-modellen diskuteras och osäkerheterna belyses kvalitativt. Generellt sätt väljs dessa värden pessimistiskt för att inte underskatta radionuklidernas utsläppshastighet. Detta angreppssätt kombinerat med de olika valda beräkningsfallen bedöms belysa effekterna av såväl osäkerheter i processer och händelser som påverkar systemets tillstånd såväl som i kvantitativa data som beskriver dessa tillstånd. Biosfärsmodellen tillåter probabilistiska beräkningar och osäkerheterna i indata till modellen kvantifieras genom att välja min-, max- och medelvärden samt formen på sannolikhetsfördelningen.

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1 Introduction

This report compiles the data selected for the migration analyses conducted within the SAFE project and is thus one of the supporting documents ("key references") to the SAFE safety assessment report. The report and the data presented herein, build on several analyses reported in other documents.

1.1 Background and aims

The SFR-1 repository for final disposal of low level radioactive waste produced at the Swedish nuclear power plants and low level waste from industry, medicine and research obtained operational license in March 1988. The aim of the project SAFE (Safety Assessment of Final Disposal of Operational Radioactive Waste) is to update the 1987 /SKB, 1987/ and 1991 /SKB, 1991/ safety analyses of SFR-1 and to prepare a safety report by the year of 2001.

SAFE is divided into three phases: (i) a pre-study, (ii) supporting analyses, and (iii) safety analysis with radionuclide migration calculations. The supporting analyses include scenario and process model identification, evaluation and modelling of inventory, evolution of the repository (near-field), evolution of the rock (far-field) and evolution of the biosphere. These analyses result in a selection of scenarios and models /SKB, 2001b/ for the assessment calculations to be carried out in the last phase. The analyses also produce the data base from which to select the input data and calculations cases to be analysed in the last safety assessment phase. These data are compiled and selected in the current report.

1.2 Objectives and scope

The overall objective of the present report is to provide the input data ("*data freeze*") to the consequence analyses to be carried out in the safety assessment stage of the SAFE project. More specifically:

- the data concern the input data for the modelling of the migration of the radionuclides (and chemotoxic substances if any) identified in the inventory of the waste or other repository components,

- data are provided both for the Base Scenario and for identified other scenarios,

- data values should always be motivated and motives should either be sufficiently provided in the current report or properly (traceably) referenced to the underlying analyses,

- if data from a single source of analyses are used in many different analyses, all these analyses should generally use the same data – exceptions need to be motivated,

- the data selection should reflect uncertainties, should not lead to an underestimation of future consequences but should not either lead to an unreasonable overestimation of the future migration of radionuclides (and other toxic substances) from the repository.

Of these points, the uncertainty treatment requires specific consideration. This is discussed in the next section.

There are also some limitations in the scope of the work presented in this report as there are aspects of overall data selection that are treated in other reports. These limitations are:

- The report does not motivate scenarios or models. This is done in the scenario report /SKB, 2001b/ and in the Main Safety Assessment report /SKB, 2001a/.

- The report does not discuss numerical discretisation or other numerical approximations needed. This means that data may be provided in this report with a higher resolution than actually used in calculations. Discretisation, approximations and their rationale are discussed in different calculation/modelling reports.

1.3   Treatment of uncertainties

Safety assessments need to consider uncertainties /NEA, 1997, SKB, 1999a/. Uncertainties originate from many sources such as incomplete knowledge of the system description or its future environment (*scenario uncertainty*), uncertainty in the description/modelling of identified processes (*conceptual uncertainty*) or uncertainty in data (*data uncertainty*). In addition, many properties, both of the rock and of the waste form, exhibit *spatial variability* and some properties may also *vary in time*. Even if the analyses aim at reducing uncertainties, some uncertainties will always remain. The impact of the uncertainties needs to be factored into the safety assessment. Uncertainties related to scenario and model selection are discussed and handled in the scenario report /SKB, 2001b/, but in order to handle data uncertainty and spatial variability it is necessary to develop some criteria for data selection.

The data selection should reflect uncertainties, should not lead to an underestimation of future consequences but should not either lead to an unreasonable overestimation of the future migration of radionuclides (and other toxic substances) from the repository. Furthermore, data should also be selected such that the safety assessment can provide guidance on which uncertainties have the largest impact on the consequences, but at the same time it is an advantage if the number of calculation cases could be reduced.

One way of handling uncertain data is to carry out probabilistic analyses and to estimate the radiological risk. A full probabilistic assessment implies estimating joint probability distributions for all model parameters. However, for many of the parameters uncertainties can only be described as intervals and the correlation between parameters could only be described in a qualitative fashion. The situation is further complicated by the fact that most repository properties and the biosphere evolve with time making the correlation between parameters quite complex. Instead the following approach is adopted:

- all selected values need to be justified either directly or through a reference,

- the selection of data is based on the performed analyses of the evolution of the repository and the description of the initial state of the repository,

- if different analyses uses the same parameter the same values should be used in these analyses, unless it can be justified why different values should be used (consistency),

- uncertainty in provided values should always be discussed and when possible be quantified,

- for each scenario the migration calculations will be based on a case where the primary data selection criteria are to strive for "reasonable" and consistent data, but simplifications leading to overestimate of releases are allowed,

- if the uncertainty in a specific data value is judged to have a large and detrimental impact on migration alternative (variant) input data are suggested.

The selection of reasonable data essentially follows the approach developed by Andersson /1999/ for the SKB SR 97 assessment /SKB, 1999a/. A reasonable value should be based on model analyses or measurements, which are:

- plausible building on the present understanding of the phenomenon, where processes known (or generally thought) to have an impact are included,

- based on actually available data,

- consistent, i.e. simultaneously consider parameters which are dependent, such that reasonable data for the different involved parameters are not in conflict with each other.

These principles should lead to a good illustration of the performance of repository for the scenario analysed. It should also be noted that all supporting analyses principally are of this character. Still, the adoption of all the above points is not completely straightforward:

- When selecting from spatially varying data the spatial resolution selected should consider the impact (i.e. the scale of the problem),

- The properties of the system components vary in time (groundwater flow, waste form degradation etc.). All aspects of the time variation cannot be captured in the migration analysis. Sensitivity analyses may be needed in order to find which simplifications are permissible.

- If simplifications in supporting analyses and migration models are needed data should be selected such that they overestimate the release from the repository.

One way of bounding the impact of uncertainty would be to select a "pessimistic" estimate of a parameter value. Pessimistic input data implies a selection of parameter values (and conceptual models) within the uncertainty range, which maximises the consequence. However, when assessing a complex time evolving system like the SFR repository it is not a priori evident which conditions that gives the maximum consequences.

Furthermore, different consequences may be differently affected by different conditions. For example, conditions leading to high releases at early times may not necessarily lead to the highest individual dose. Still in selecting reasonable parameter values it can sometimes be obvious that selecting another value within the uncertainty range would lead to higher releases or facilitated migration. In such cases alternative values will be suggested. These values will then be used in the final safety assessment in order to illustrate the significance of the relevant uncertainties.

1.4   Structure of report

The selection of scenarios and calculation cases for quantitative analyses are described in Chapter 2 together with the expected evolution of barrier properties and conditions. A short description of the migration models is given in Chapter 3 in terms of the data

required by each model. The repository design and waste characteristics are given in Chapter 4 and the hydrogeology in the engineered barriers and the derivation of data to the migration calculations are addressed in Chapter 5. In Chapter 6 the chemical and physical data for the engineered barriers are discussed and compiled. Selected data for calculating the migration in the geosphere are given in Chapter 7 and in Chapter 8 all data selected for calculations of the biosphere migration and resulting dose rates are compiled.

2   Scenarios and calculation cases

A systematic scenario and system analysis has been conducted within the SAFE project and the results are given in a separate report /SKB, 2001b/. The report generally documents and justifies the selected system description model, selected scenario initiating events and conditions, the general selection of the type of quantitative evaluation models to be used and the information flow between models. The outcome of this work together with other supporting analyses form the basis for the selection of calculation cases and input data to the quantitative assessment of radionuclide release from SFR-1. In this Chapter, the selected scenarios and calculation cases are described.

2.1   Base Scenario

2.1.1   Scenario definition

The starting point for the scenario analysis within SAFE is the selection of a Base Scenario. The Base Scenario should be highly plausible and be a good reference point for superposition with scenarios other than the base scenarios. In essence the Base Scenario assumes that the repository at closure is constructed according to specification and that the external environment will stay the same, although well known trends, such as land rise will be included in the scenario.

The general assumptions that defines the Base Scenario are /SKB, 2001b/:

- The state of barriers and plugs at repository closure is in accordance with design criteria.

- Present day climate maintains for 10 000 years after repository closure.

- The best estimate of the future land rise is considered.

- The types of ecosystems in the biosphere system are the same as those present today, but succession due to land rise is considered.

- Present day wells and future wells that do not penetrate the repository barriers are considered.

- The time considered for the evolution of the system is restricted to 10 000 years.

The development of a qualitative system description model for the Base Scenario has revealed a number of processes that are expected to contribute to the evolution of the characteristics of the disposal system /SKB, 2001b/. The expected evolution and assumed characteristics of importance for the release and migration of radionuclides are summarised in the following sub-sections as a background to the selected calculation cases.

2.1.2   Repository evolution

The characteristics of main importance for the release and migration of radionuclides in the engineered barriers in the repository are the permeability and chemical properties of the barriers as well as the hydrogeochemical conditions. In addition, the hydrogeological and hydrogeochemical conditions in the surrounding rock is of importance (see Section 2.1.3) as well as gas generation in the repository that via expulsion of water can accelerate the release of radionuclides.

Hydrogeochemical conditions

The redox potential, pH and salinity of the water in the engineered barriers in the different repository parts as well as its content of complexing agents and colloids are of great importance for the performance of the barriers in retaining the release of radionuclides. Processes that will affect these entities are mainly /SKB, 2001b/:

- Metal corrosion and microbial activity that will consume oxygen and establish reducing conditions after repository closure and water saturation.

- Dissolution (leaching) of cementitious components from the concrete barriers and reactions with minerals in bentonite barriers and rock fill that will determine the pH of the water and affect the ionic strength.

- Dissolution of chemicals in the waste and degradation of organic materials that together with sorption on cement will affect the content of complexing agents.

- Formation and stability of colloids that in turn is dependent on e.g. the ionic strength of the water

- Diffusion, advection and mixing that will determine the temporal and spatial distribution of dissolved species.

In an assessment of the long-term degradation of concrete in SFR /Höglund, 2001/ it is concluded that the expected chemical changes are slow and that alkaline conditions will be maintained in the concrete during the entire period of 10 000 years. In case of diffusion dominated transport in the pore water of the concrete and fast exchange of groundwater outside the concrete, pH might drop to a value between 11 and 12 after 1000 years of leaching in the outermost 5 to 10 cm of the concrete. After 8000 years the zone with a pH below 12 might have reached about 0.2 m into the concrete and after 10 000 years about 0.4 m into the concrete. If the concrete is fractured and advective transport with percolating water is dominating the leaching is faster. However, the pH will not drop below 10 even in the most degraded parts of the concrete within 10 000 years of water percolation with a specific flow of about 0.007 m/year /Höglund, 2001/. This specific flow corresponds to one porewater exchange in 15.5 years. After 1000 years the pH is above 12 in all parts of the concrete except in the first 0.2 m of the concrete at the upstream side. In a concrete barrier surrounded by sand/bentonite, only very small changes in pH are expected over the entire time period of 10 000 years /Höglund, 2001/.

A rough indication of the potential changes in composition of pore water and mineralogy can be obtained from the calculations of the hydrogeochemical interaction between concrete and sand/bentonite that have been carried out by Höglund /2001/. In these calculations the hydrogeochemical interaction between the concrete lid in the Silo and the sand/bentonite above the lid and groundwater is modelled. The results indicate that chloride intrusion from the groundwater will decrease the initial pH in the sand/bentonite down to about pH 9 close to the interface with the groundwater, but this decrease is followed by an increase in pH in response to alkaline components from the concrete. In the sand/bentonite close to the concrete the influence of the alkaline components in the concrete results in a fast increase in pH to values above 12. It should be noted that possible chemical effects of the alkaline concrete water on the stability of montmorillonite, e.g. alkaline hydrolysis, not are included in these calculations. If such reactions occur, the pH may be affected, but the most reasonable assumption still seems to be that the pH in the pore water of both the bentonite and the sand/bentonite barriers in the Silo may well be above 10.

Chemicals in the waste can dissolve and form complexes with radionuclides and complexing agents can also be generated when materials in the waste are degraded, e.g. the formation of isosaccharinic acid by alkaline degradation of cellulose. Based on an inventory of chemicals and cellulose materials in the waste the concentration of complexing agents in the different waste types has been estimated /Fanger *et al*., 2001/. These estimates show that it cannot be excluded that the concentration of some complexing agents is close to the level where some impact on sorption could be expected. However, since these concentrations are obtained inside the waste packages and only for a few waste types, mostly waste conditioned in bitumen, it is judged that the effect of complexing agents is implicitly considered in the rather conservative choice of sorption data in the Base scenario (see Section 6.2).

Based on the analyses carried out and on qualitative assessments the following hydrogeochemical conditions are assumed for the repository in the Base Scenario:

- Reducing conditions will be established and maintained over the whole time period of 10 000 years in all the repository vaults.

- A pH above 12 will remain over the whole time period of 10 000 years in the concrete barriers in the Silo as well as in the internal parts of the concrete barriers in the BMA and BTF vaults. In the outermost parts of the concrete lid and walls in BMA and in the concrete lid and concrete grout in the BTF vaults, a pH drop down to values around 11 can occur after long times. The water in the bentonite and sand/bentonite barriers in the Silo and in the rock fill in the BMA and BTF vaults is expected to have a pH in between the pH of the intruding groundwater and the pH of the concrete water. The pH of the water in the BLA vaults is expected to be the same as the pH of the intruding groundwater.

- The amount of colloids in the engineered barriers in the Silo and in the BMA and BTF vaults is assumed to be negligibly small, since the concrete barriers will supply calcium ions. Furthermore, the calcium content of the intruding groundwater is high, which should prevent extensive colloid formation also in BLA, which has no concrete barriers.

- Dissolution of chemicals in the waste and degradation of waste materials can in some waste types result in such concentration levels of complexing agents that sorption inside the waste packages can be affected.

- The water in all repository vaults is assumed to have a high content of dissolved salts (high ionic strength) over the whole time period of 10 000 years, despite that the groundwater in the future is expected to become more fresh. This assumption is pessimistic for the choice of e.g. sorption data (see Section 6.2).

Barrier properties

The permeability of the engineered barriers to both water and gas will affect the release of radionuclides from the repository vaults. The permeability is mainly determined by the geometry, porosity and fracture characteristics of the barriers. In addition, the chemical composition of the barriers can affect sorption and thus the retention of radionuclides in the repository barriers.

At repository closure, the *concrete barriers* in the repository vaults may contain small fractures that are formed during the operational phase, e.g. due to thermal stresses from cement hydration, drying shrinkage and settlement due to movement of underlying

materials. Processes that will affect the properties after repository closure are mainly /SKB, 2001b/:

- Dissolution (leaching) of cementitious components and formation of reaction products.

- Cracking/deformation due to the formation of volume expanding reaction products e.g. ettringite and corrosion products, and due to the creation of gas overpressure, e.g. due to hydrogen evolving corrosion.

The leaching of the concrete barriers in saline groundwater and the complex chemical interactions between the cement minerals of the concrete and species in the water has been quantitatively studied by numerical modelling /Höglund, 2001/. The calculation show that the porosity of fully hydrated structural concrete of the type used in SFR is about 10 %. Due to the chemical reactions that will take place after saturation with groundwater, the porosity will at most increase to 19 % and decrease to about 6 % in the cases studied. If the exchange of reacting components is diffusion limited the largest change in mineral composition and porosity will take place close to the interface between concrete and moving groundwater. At larger distances from the moving groundwater the change is smaller and at a depth of 0.4 m and larger the porosity will decrease to about 8 % after 3000 years and after that remain at that level for the rest of the time period. At these depths the calcium silicates of the concrete remain essentially intact even after 10 000 years, while formation of Friedelsalt and an accompanying reduction of the amount of portlandite due to chloride intrusion from the groundwater are predicted. If instead the exchange of reacting components is controlled by water percolating through the concrete at a rate corresponding to one porewater exchange in 15.5 years, significant mineral transformations are predicted to occur throughout the whole of a 1 m thick concrete slab. The calcium silicates of the concrete are almost depleted to a depth of 0.3 to 0.4 m in the direction of the percolating water after 10 000 years. The initial porosity of 10 % decreases to minimum value of about 8 % and increases thereafter to a maximum value of about 17 % along with the moving leaching front. Even after 10 000 years, only small changes in porosity and mineral composition are predicted for a concrete surrounded by a sand/bentonite barrier.

Components dissolved from the waste and products from degradation of materials in the waste can also react with cement minerals in the concrete barriers. Sulphate from ion-exchange resins can cause formation of ettringite, carbon dioxide from degradation of organic materials can via dissolution in the concrete water precipitate as calcite, and any sulphate as well as carbonate and chloride that are released from evaporator concentrates in bitumen can react with cement minerals. Furthermore, corrosion of metals in waste and barriers will generate gas and volume expanding corrosion products. These processes have not been quantitatively analysed, but earlier analyses of SFR and qualitative assessments of the potential impact of these processes indicate that cracking of the concrete barriers not seems very likely. On the other hand it cannot be totally excluded and therefore the impact of fractured concrete barriers in the Silo, BMA and BTF vaults is analysed in one calculation case defined for the Base Scenario.

Concrete waste packages and cement grout in packages will after repository closure be exposed to similar processes as the concrete barriers. However, the modelling reported by Höglund /2001/ indicates that no leaching will occur within 10 000 years. However, fracturing due to e.g. ettringite formation caused by sulphate from ion exchange resins or due to creation of high internal gas pressure cannot be excluded. Therefore the impact of fractures in concrete packages and cement grout in packages is implicitly considered in one of the calculation cases defined for the Base Scenario.

At repository closure, the *steel packages* in the repository vaults may be water tight, but some of them may also be permeable to water. Anyhow, corrosion will in time make all steel packages permeable, and the corrosion products that are formed may act as sorbents for some radionuclides. In the analysis of the Base Scenario the steel packages are not considered as any barriers to water intrusion or release of radionuclides and the potential sorption on corrosion products is neglected.

The main changes in a *bitumen waste matrix* after repository closure is expected to be due to water uptake and swelling /SKB, 2001b/. A characterisation of the bitumenised waste in SFR /Pettersson and Elert, 2001/ indicates that the release of radionuclides from waste in bitumen can be significantly delayed due to the time required for water uptake and creation of connected transport paths in the bitumen matrix. This is considered in the analysis of the Base Scenario by assuming that the release of radionuclides in waste contained in bitumen will be distributed over a time period of 100 years /Lindgren *et al.*, 2001/.

At repository closure, the *bentonite* and *sand/bentonite* barriers in the Silo are expected to have a permeability as well as sorption property that are related to the density and composition of the barriers. Processes that will affect the properties after repository closure are mainly /SKB, 2001b/:

- Transformation of the montmorillonite in the bentonite barriers. For example, the presence of potassium may lead to formation of illite and high pH may lead to alkaline hydrolysis of montmorillonite.

- Dissolution/precipitation of non-clay minerals and other impurities in the bentonite barriers.

- Ion exchange, where sodium in the bentonite is replaced by potassium, calcium and magnesium supplied by the concrete and dissolved in the groundwater.

- Bentonite expansion and dispersion of clay particles.

Ion exchange with calcium, potassium and magnesium both from the groundwater and from the concrete is included in the hydrogeochemical modelling carried out by Höglund /2001/. Ion exchange will gradually convert the sodium bentonite to calcium, potassium and magnesium bentonite. In addition, the modelling results showed precipitation of brucite and calcite and also some ettringite closest to the interface between the concrete and the sand/bentonite. The impact of high pH on the properties of bentonite and sand/bentonite has not been quantitatively analysed. However, the present knowledge indicates that the low temperature in the bentonite around the Silo will prevent extensive transformation to illite in a time perspective of 10 000 years. A high pH will probably cause a dissolution of accessory minerals in the bentonite buffer rather than alkaline hydrolysis of the montmorillonite. This is supported by results from experiments where sodium bentonite was percolated with calcium hydroxide (pH = 13.8) during 16 months /Karnland, 1997/. Only small changes in the bentonite was observed in terms of dissolution of cristobalite and silica and formation of CSH phases and minor formation of illite, but no clear evidence of montmorillonite alteration was found. Because of the uncertainties associated with the impact of concrete pore water on bentonite, changes in hydraulic properties of these barriers in the Silo is implicitly considered in a calculation case for the Base Scenario. Potential changes in sorption properties is neglected since it is judged that the reaction products formed would be at least as good sorbents as the original minerals (see Section 6.2.2).

At repository closure, the *rock fill* in the repository vaults is assumed to have a rather high permeability and sorption properties typical for Swedish granite. The main process that will affect the properties after repository closure is judged to be chemical alteration due to the impact of concrete pore water /SKB, 2001b/. Concrete pore water may react with the rock fill thereby possibly changing the properties of the fill, e.g. porosity and sorption capacities. Calcite and brucite may precipitate in the void and secondary calcium silicate hydrate (CSH) phases that form on the surface of the solid material may lead to some volume increase in the solid phase and thereby reduced porosity. These potential changes are not explicitly treated in the analysis of the Base Scenario, but are discussed and considered in the selection of data (see Section 6).

Gas generation and release

Gas can be generated in the repository through anaerobic corrosion of metals, through microbial degradation of organic materials and possibly also through radiolytic decomposition of water and organic materials. The potential gas generation in the different repository parts and the impact of gas mediated release of dissolved radionuclides are studied within the Base Scenario /Moreno *et al.,* 2001/.

2.1.3   Geosphere evolution

The capacity of the geosphere to delay the transport of radionuclides released from the repository depends on the transport resistance of the rock. The main features that affect the transport resistance are the magnitude of the groundwater flow, the length of the transport paths and the exchange of radionuclides between flowing water and the rock in contact with this water. This exchange is in turn dependent on groundwater composition and properties of the rock.

The progressive land rise and shore line displacement is expected to be the main cause for future changes in groundwater flow and length of transport paths. This will also in the future cause a change in groundwater composition from the present saline groundwater to a groundwater with less content of dissolved salt. There are also other processes in the geosphere that may change the properties of the rock and water, at least locally, such as reactions between components from the repository and rock minerals. In addition, transport by colloids may enhance the migration of radionuclides in the geosphere. The impact of land rise on groundwater flow and water flow through the repository is considered in the analysis of the Base Scenario, while the impact of future changes on radionuclide migration in the geosphere is indirectly considered by defining two simple calculation cases. In one of the cases, the geosphere is totally neglected as a barrier for radionuclides and in the other case it is assumed that the migration parameters in the geosphere are constant in time and representative for the present conditions in the rock around SFR.

2.1.4   Biosphere evolution

The three main factors that will affect the evolution of the biosphere are the progressive land rise and accompanying shore level displacement, future changes in climate and internal slow processes like vegetation succession and overgrowing of lakes. The effects of land rise and internal processes are considered when developing a conceptual model of a reasonable biosphere evolution in the area, while climatic factors belong to the group of other scenarios analysed (see Section 2.2).

The reasonable biosphere evolution is defined based on a number of analyses carried out and is described in Kautsky /2001/. In summary, the reasonable evolution is defined as the release of radionuclides to a coastal recipient from the time of repository closure until year 5000 AD. The present conditions in that part of the Öregrundsgrepen are

assumed to prevail until year 4000 AD, but the water volume and water exchange is smaller from year 4000 AD due to the effect of land rise and shore level displacement. From 5000 AD to 8000 AD, radionuclides are released to a lake that has developed in the area. The characteristics of the lake are the same as those that defines lakes in the area today. At year 8000 AD the lake is overgrown and wetlands and mires have developed. It is assumed that these are drained and used for agricultural purposes in the time period 8000 AD to 12 000 AD.

An alternative case is defined in order to illustrate uncertainties in the location of discharge areas for groundwater and radionuclides. In this case it is assumed that the discharge take place to a mire from 4000 AD to 12 000 AD. In addition, the consequence of a well drilled downstream the repository should be part of the Base Scenario as well as the consequences of maintaining the present biosphere conditions in the discharge area over the whole time period.

2.1.5   Calculation cases

Based on the expected evolution of the repository, geosphere and biosphere calculation cases for the Base Scenario are defined. A short description of these calculation cases are given here, while more detailed descriptions are found in the report presenting the analysis of radionuclide release and dose /Lindgren *et al.*, 2001/ and in the report analysing the consequence of gas generation on the release of radionuclides /Moreno *et al.*, 2001/.

The calculation cases that are defined for the Base Scenario are:

Intact engineered barriers

The state of all engineered barriers is in accordance with design criteria at repository closure. The barrier properties remain unchanged for the whole time period considered in the analysis, while the water flow in the barriers and repository vaults will change due to the on-going land rise.

Two alternatives for the treatment of the geosphere migration are defined. Either the impact of retardation of radionuclides in the geosphere is neglected or the retardation is considered by the use of constant migration parameters for the whole time period.

Radionuclide turnover in the biosphere and resulting dose to man is estimated for a "Reasonable biosphere evolution", but also for the release to a mire and for the release to a well located downstream the repository. In addition, the consequences of release to Öregrundsgrepen with the present conditions remaining over the whole time period are illustrated.

Impact of gas

Expulsion of water containing radionuclides from the interior of the Silo, BMA and BTF vaults due to gas generation and pressure build-up. Otherwise the same conditions as defined for the case denoted Intact engineered barriers.

Degraded engineered barriers

All conditions are the same as defined for the case denoted Intact engineered barriers from the time of repository closure (2000 AD) until 3000 AD. From 3000 AD and onwards it is assumed that the hydraulic conditions in the repository vaults are changed due to fracturing/degradation of the barriers. Other conditions in the repository vaults, geosphere and biosphere are the same as those defined for the case denoted Intact engineered barriers.

2.2   Other scenarios

In the scenario and system analysis of SFR, a number of other scenarios was selected and qualitatively assessed /SKB, 2001b/. This resulted in a few other scenarios that should be included in the quantitative analysis of radionuclide release from the repository. The calculation cases defined for the scenario initiating events or conditions that should be analysed are briefly described in the following subsections. More detailed descriptions are given in other reports /Lindgren *et al.*, 2001 and Moreno *et al.*, 2001/.

2.2.1   Initial defects in technical barriers

The conditions that should be evaluated in terms of initial defects are defects in engineered structures and undesirable materials left in the repository /SKB, 2001b/. Defects in engineered structures are addressed as fractures in concrete structures and improper/defect plugs. Undesirable materials left in the repository is assessed as the presence of chemicals/complexing agents in the repository that affects the sorption of radionuclides.

Fractures in concrete structures

Fracture(s) are present in the concrete structures at repository closure. This give higher water flow through the engineered barriers compared with the case in the Base Scenario denoted "Intact engineered barriers". Otherwise the conditions are the same as those defined for the case denoted "Intact engineered barriers" in the Base Scenario.

Fractures in concrete structures and gas generation

Expulsion of water containing radionuclides from the interior of the repository vaults through fracture(s) in the concrete structures due to gas generation and pressure build-up. Otherwise the conditions are the same as those defined for the case denoted "Fractures in concrete structures".

Improper/defect plugs

Improper/defect plugs in the access tunnel and in the repository vaults can affect the hydraulic situation in the repository vaults. The consequence of defect plugs on the magnitude and distribution of the groundwater flow in the repository vaults has been analysed by Holmén and Stigsson /2001a/. However, the design of the plugs is not yet finally decided and it is therefore not meaningful to carry out a detailed analysis of the release of radionuclides. The results from the hydrogeological analyses can be used to give an indication on the impact of improper plugs. This is done and the results are given and discussed in the main safety report /SKB, 2001a/.

Chemicals/complexing agents and intact engineered barriers

Lower sorption is assumed in the engineered barriers of radionuclides that are affected by the presence of complexing agents. Otherwise the conditions are the same as those defined for the case denoted "Intact engineered barriers" in the Base Scenario.

Chemicals/complexing agents and degraded engineered barriers

Lower sorption is assumed in the engineered barriers of radionuclides that are affected by the presence of complexing agents. Otherwise the conditions are the same as those defined for the case denoted "Degraded engineered barriers" in the Base Scenario.

2.2.2 Climate change

The climate related events and conditions are by a qualitative assessment judged to be well covered by the analyses defined for the Base Scenario /SKB, 2001b/. Despite this it is recommended that a separate analysis is carried out to illustrate the consequences of a future development of continuous permafrost in the area /SKB, 2001b/. Based on the expected future climate evolution it is judged that the development of permafrost in the Forsmark area within the coming 10 000 years is quite unlikely. If it at all occurs it will most likely be discontinuous, i.e. with patches of frozen ground surrounded by unfrozen ground. Effects of discontinuous permafrost are well covered by the assumptions already made within the Base Scenario /SKB, 2001b/. The extremely unlikely event of continuous permafrost could only start at the end of the assessment period, otherwise the time for freezing and thawing would be far too short /SKB, 2001b/.

Permafrost

A very simple calculation case is defined where the repository is considered as frozen until 12 000 AD when all radionuclides are released with the total groundwater flow that passes through the repository vaults. The radionuclide turnover in the biosphere and resulting dose to man are estimated for the biosphere conditions that prevail today.

2.2.3 Human activities

There are a large number of human activities that could be relevant for the SFR repository area, but the consequence of a well drilled into the repository is chosen as a representative scenario for human activities /SKB, 2001b/.

Intrusion well

A well is drilled into the different repository vaults when the shoreline has passed beyond the repository area and it is possible to drill wells into the repository vaults. Humans are exposed to radionuclides by drinking water from the well.

The presence of the well also affects the hydraulic situation in the vaults and the well could act as a fast transport route for radionuclides from the repository to the surface. These long-term effects of an intrusion well is not included in the calculation case, but are discussed in the main safety report /SKB, 2001a/.

3 Migration models

3.1 General

The SAFE evaluation of radionuclide transport is made with a series of coupled models, which in turn require input from analyses of the state of the barriers, the rock and the biosphere. This chapter briefly describes the models and the data needed as input to the models as a background to subsequent chapters where the selected input data are compiled. More detailed descriptions of the models are given in the report on the analysis of radionuclide release and dose /Lindgren *et al.*, 2001/ and in a separate report describing the biosphere model /Karlsson *et al.*, 2001a/.

3.2 Repository vaults - Near field

3.2.1 Migration code

The near-field code NUCFLOW is a compartment model developed from the NUCTRAN-code /Romero, 1995 and Romero *et al.*, 1999/. NUCFLOW is a multiple path model that calculates the instationary nuclide transport by diffusion and advection considering sorption and radioactive chain decay.

In the model, each vault is divided into a number of compartments. Transfer of radionuclides between the compartments and out to the surrounding rock occurs by diffusion and advection. The advective transport is determined by the direction and magnitude of water flow between and out from the compartments. The diffusive transport out to the groundwater flowing in the surrounding rock is calculated from the Darcy velocity in the rock. Within each compartment the code keeps track of the amount of radionuclides, and calculates the concentration in the available water while considering linear sorption and solubility limits.

The compartments are defined by their volume, their diffusion length and cross sectional area available for diffusion and by their material data, such as porosity and density.

3.2.2 Data requirements

In summary the code generally requires the following input data:

- Geometry and dimensions of the waste packages, engineered barriers and repository vaults

- Quantity of different materials and material data, such as porosity and density, of the materials in waste packages and engineered barriers

- The initial inventory and half-lives of radionuclides in the waste

- Dissolution rate and solubility of radionuclides

- Sorption coefficients (K_d-values) for radionuclides in the different materials

- Diffusivity of radionuclides in the different materials

- The magnitude and direction of water flow in different parts of the repository vaults

- The Darcy velocity (groundwater flux) in the surrounding rock

3.3 Geosphere – Far field

3.3.1 Migration code

The far field code FARF31 /Norman and Kjellbert, 1990/ is a one-dimensional model for calculating the migration of radionuclides along a single flow path in the geosphere. The model considers advection and dispersion along the flow path, diffusion and sorption in the rock matrix transverse the path and radioactive chain decay. Dispersion is described with a constant dispersivity and expressed as a Peclet number. Retardation in the rock is dependent on the flow velocity in the fracture, which is described with the travel time t_w and the F factor, which takes into account the exchange between nuclides in the water and in the rock matrix. The F factor can be expressed as the product of the advective travel time and the flow-wetted surface area per volume of water in the transport pathway ($t_w \cdot a_w$), but other descriptions are also possible, see e.g. /Andersson *et al.*, 1998/. In order to describe matrix diffusion and sorption in the rock's micropore structure, information is required on matrix diffusivity (D_e), matrix porosity (ε_r), maximum penetration depth and sorption values (K_d) for the different nuclides.

3.3.2 Data requirements

The direct input parameters to the model are:

- The advective travel time in the geosphere. This is a theoretical quantity used to transfer results from the hydrogeological models to migration models. It could be seen as the transport time in the geosphere for a particle moving with the same velocity as the groundwater without interacting with the rock.

- The Peclet number

- The flow-wetted rock surface area per volume of flowing water

- The rock matrix porosity and maximum penetration depth into the rock matrix by diffusion

- The effective diffusivity (D_e) of radionuclides in the rock matrix

- The sorption coefficient (K_d) of radionuclides in the rock matrix

- The half-lives of radionuclides

3.4 Biosphere

3.4.1 Code

The compartment model ACTIVI/PRISM /Bergström *et al.*, 1982 and 1995 and Gardner *et al.*, 1983/ is used to simulate the transfer of radionuclides in the biosphere and to calculate the dose to humans. It considers the distribution of radionuclides between major physical components of the biosphere in terms of transfer coefficients or rate constants. Important processes considered in the derivation of transfer factors are water turnover, erosion, sedimentation and resuspension, bioturbation, sorption, and radioactive decay.

Uptake in aquatic biota is calculated using bioaccumulation factors whereas uptake in terrestrial vegetation is simulated using root-uptake factors and translocation factors (for radionuclides added to the vegetation surface). Specific transfer factors are used to calculate the transfer of radionuclides to milk and cattle meat.

The internal exposure of humans is a combination of exposure from radionuclides that are eaten and those that are inhaled. Exposure from the former ones is calculated by combining the concentration in food, consumption rates and nuclide specific dose coefficients for conversion from activity to dose for ingested radionuclides. Exposure via inhalation is calculated from radionuclide concentration in air, inhalation rates and nuclide specific dose coefficients for conversion from activity to dose for inhaled radionuclides. External exposure is estimated through consideration of exposure times, concentration of radionuclides in the air or on the ground and nuclide specific dose coefficients for conversion from concentration of radionuclides to dose for external exposure.

3.4.2 Data requirements

The biosphere model requires data on the following sets of parameters (for more details see Section 8.2):

- Geometrical parameters (areas, depths etc of the different physical components)

- Physical/chemical parameters (water flows, sorption coefficients etc)

- Biological parameters (root uptake factors and bioaccumulation factors, translocation factors etc)

- Living habits of humans and cattle (irrigation, consumption patterns etc)

- Radiological parameters (dose conversion factors, half-lives of radionuclides)

The model system allows for probabilistic calculations. This means that a best estimate value as well as minimum and maximum values and the distribution function are required as input.

4 Repository and waste

4.1 General

In this chapter data and information on repository design and waste inventory used in the safety analysis are compiled. More details on the derived waste inventory are given in Riggare and Johansson /2001/ and a detailed description on repository lay-out and design can be found in the main report /SKB, 2001a/ and in construction drawings /Forsgren, 1987/

The SFR-1 repository is located in the vicinity of Forsmark nuclear power plant, about 160 km northeast of Stockholm. SFR-1 is situated in crystalline bedrock at a depth of more than 50 metres below the seabed, which is in turn under 5 metres of water.

SFR-1 is the facility for final disposal of short-lived low- and intermediate- level waste from the Swedish nuclear power plants and from the central interim storage for spent nuclear fuel (CLAB), and similar radioactive waste from medical care, industry and research. The waste is located to different repository parts depending on the type of waste and its activity content. At present SFR-1 consists of the Silo and four vaults denoted BMA, BLA, 1BTF and 2BTF. An overview of the underground facility is shown in Figure 4-1.
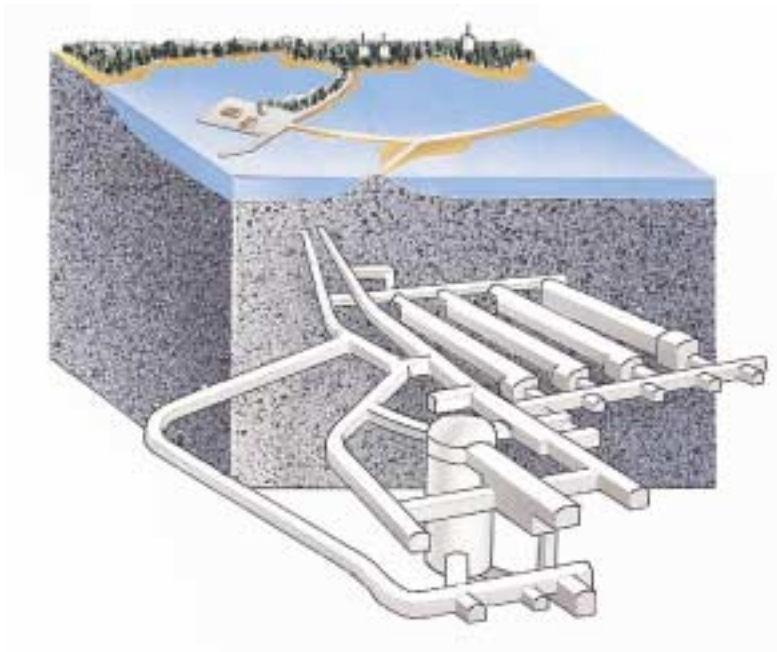
Figure 4-1. *Overview of the SFR-1 repository*

4.2 Repository parts and dimensions

Data regarding the construction of the repository parts and the waste located to them that are needed for the modelling of the migration of radionuclides from the repository is presented in the following sections.

4.2.1 Data sources

Data given in this section is taken primarily from three different sources. Data on the dimensions of the repository parts are from a compilation of data used for the radio-nuclide transport calculations for SFR in a previous safety assessment /Wiborgh and Lindgren, 1987/ and from construction drawings /Forsgren, 1987/. Data regarding the waste and the waste packaging are taken from a recent waste characterisation study /Riggare and Johansson, 2001/.

Silo

The Silo consists of a concrete cylinder with a height of about 53 m and an outer diameter of about 28 m. The thickness of the concrete walls is 0.8 m and the concrete bottom plate is 1 m thick. The interior of the concrete cylinder is divided into vertical shafts with intervening concrete walls, 0.2 m thick. The waste packages are placed in the shafts and the voids between the waste packages are gradually backfilled with concrete grout. Each shaft takes 42 layers of concrete/steel moulds or 56 layers of steel drums. The majority of the shafts have a squared cross-section 2.55 x 2.55 m adapted to contain four moulds or 16 drums in each layer.

The slot between the cylindrical concrete walls and the surrounding rock is filled with bentonite, on average 1.2 m thick. The concrete cylinder is resting on a 1.5 m thick mixture of 10% bentonite and 90% sand by weight.

According to present plans, the sealing of the Silo will be carried out by placing a 1 m thick concrete lid on top of the concrete cylinder. The lid can be equipped with evacuation pipes in order to allow escape of gas that is generated inside the concrete cylinder. The top of the lid will be covered by a thin layer of sand (about 100 mm) and a 1.5 m thick mixture of 10 weight % bentonite and 90 weight % sand. The remaining void above the mixture of bentonite and sand will be filled with sand or gravel or with sand stabilised in cement /SKB, 1998/. The silo dimensions are compiled in Table 4-1.

The Silo is designed for approximately 18 500 m^3 of conditioned waste (SKB, 1998). Most of the waste, about 98 %, is ion-exchange resins and the remaining 2 % are scrap and trash. All of the waste is conditioned, about 80 % in cement and 20 % in bitumen.

The waste allocated to the Silo is packed in concrete moulds, steel moulds and in steel drums. The dimensions of the moulds are 1.2×1.2×1.2 m. The drums have a diameter of about 0.6 m and a height of about 0.9 m. Steel drums are placed on a steel plate or in a steel box with the same dimensions as the moulds loaded into the shaft in the Silo.

The waste allocated to the Silo can be divided into the following categories:

- Concrete moulds with waste stabilised in cement.

- Steel moulds with waste stabilised in cement.

- Steel drums with waste stabilised in cement.

- Steel moulds with waste stabilised in bitumen.

- Steel drums with waste stabilised in bitumen.

Table 4-1. Dimensions of the Silo repository

Property	Value	Reference
Silo		
Diameter [m]	*29.5 [2)]*	*Forsgren, 1987*
Diameter upper part [m]	*31 [2)]*	*Forsgren, 1987*
Height [m]	*69.5 [2)]*	*Forsgren, 1987*
Height of cylindrical part [m]	*63 [2)]*	*Forsgren, 1987*
Concrete structure (=waste storage)		
Outer diameter [m]	*27.5 [2)]*	*Forsgren, 1987*
Wall thickness [m]	*0.8 [1)]*	*Forsgren, 1987*
Floor diameter [m]	*28 [1)]*	*Forsgren, 1987*
Floor thickness [m]	*1 [1)]*	*Forsgren, 1987*
Lid diameter [m]	*26.6 [1)]*	*Forsgren, 1987*
Lid thickness [m]	*1 [1)]*	*Wiborgh and Lindgren, 1987*
Height [m]	*53 [2)]*	*Forsgren, 1987*
Height of shafts to upper edge of concrete structure [m]	*52.5 [2)]*	*Forsgren, 1987*
Inner walls height [m]	*51.3 [1)]*	*Forsgren, 1987*
Inner walls thickness [m]	*0.2*	*Wiborgh and Lindgren, 1987*
Concrete volume [m³]	*9500 [2)]*	*Forsgren, 1987*
Shaft type 1, 2.55 x 2.55 [no]	*57*	*Forsgren, 1987*
Shaft type 2, 2.55 x 1.35 [no]	*12*	*Forsgren, 1987*
Shaft type 3 [no]	*4*	*Forsgren, 1987*
Shaft type 4 [no]	*8*	*Forsgren, 1987*
Bentonite		
Height [m]	*51.8*	*Forsgren, 1987*
Thickness [m]	*1 [2)]*	*Forsgren, 1987*
	1.2	*Wiborgh and Lindgren, 1987*
Sand – bentonite (90/10)		
Floor diameter [m]	*28.8 [1)]*	*Forsgren, 1987*
Floor thickness [m]	*1.5*	*Forsgren, 1987*
Lid diameter [m]	*31*	*SKB, 1993*
Lid thickness [m]	*1.5*	*Wiborgh and Lindgren, 1987*
Sand		
Sand below concrete lid thickness [m]	*0.05*	*SKB, 1993*
Sand above concrete lid thickness [m]	*0.1*	*SKB, 1993*
Sand above concrete lid diameter [m]	*31*	*same as diameter of the upper part of the silo*
Concrete not reinforced (between sand-bentonite and gravel		
Diameter [m]	*31*	*same as diameter of the upper part of the silo*
Thickness [m]	*thin*	*SKB, 1993*
Gravel (remaining space in top of silo)		
Diameter [m]	*31*	*same as diameter of the upper part of the silo*
Thickness [m]	*max 10*	*Assumed*

1) Measured in drawings in Forsgren /1987/
2) Given as an approximate value by Forsgren /1987/

About 43 % of the waste volume consist of concrete moulds, 47 % of steel moulds and 10 % of steel drums. A short description of the waste types and the amount of each type to be deposited in the Silo are given in Table 4-2.

Table 4-2. Waste types allocated to SILO and the prognosticated number of waste packages and storage volume at repository closure /Riggare and Johansson, 2001/.

Waste type		Package type	No of packages	Storage volume [m^3]
O.02	Cement conditioned ion-exchange resins	Concrete mould (0.1 m) [1]	2094	3618
C.02	Cement conditioned ion-exchange resins	Concrete mould (0.1 m) [1]	1438	2485
C.24	Trash in cement	Concrete mould (0.1 m) [1]	135	233
C.24 drum	Trash in cement	Steel drum in concrete mould (0.1 m) [1]	15	26
R.02	Cement conditioned ion-exchange resins	Concrete mould (0.1 m) [1]	705	1218
R.16	Cement conditioned ion-exchange resins	Steel mould	3733	6451
B.06	Bitumen conditioned ion-exchange resins	Steel drum	6902	1693
F.18	Bitumen conditioned ion-exchange resins	Steel mould	938	1621
S.04	Cement conditioned ion-exchange resins	Steel drum	134	33
S.11	Cement conditioned sludge	Steel mould	96	166
S.22	Unconditioned scrap	Steel drum (100 l) in steel drum (200 l)	430	105
S.24	Trash in cement	Concrete mould (0.1 m) [1]	2	3
Total			16622	17652

1)   0.1 m refers to the thickness of the mould walls.

BMA

The rock vault for intermediate level waste, BMA, is 160 m long with a wall height of 11.5 m and a maximum height of 16.5 m and a width of 19.6 m. The waste packages are placed into a concrete structure, 140 m long and 8.4 m high and 15.6 m wide. The concrete structure is divided into 13 large compartments and two small compartments by inner concrete walls. The inner length of the large compartments in the length-direction of the vault is 9.9 m and the cross sectional inner length is 15.6 m. The two small compartments have an inner length of about 5 m in the length direction of the vault and the inner length in the cross-sectional direction of the vault is 7.2 m. Both the outer and inner concrete walls are 0.4 m thick except for the cross-sectional wall facing the reloading zone, which is 0.6 m thick. The bottom of the compartments consists of a concrete floor, 0.25 m thick, that rests on a layer of gravel.

The waste packages are piled on the concrete floor in the compartments in such a way that each compartment will have at least two rows of concrete moulds that act as a support for pre-fabricated reinforced concrete lids. The lids are put in position as soon as a compartment is filled and after that a 5 cm thick concrete layer is cast on top of the lid in order to prevent water intrusion during the operational phase.

At repository closure, an additional 0.5 m thick reinforced concrete lid will be cast on top of the compartments. The space between the waste packages inside the compartments will either be left empty or filled with the same type of concrete grout that is used as backfill material inside the Silo. The space between the concrete structure

and the rock walls, about 2 m wide on each side, as well as the re-loading zone will be filled with sand. The space above the concrete lid will either be left unfilled or will be filled with sand. In the SAFE-project it is assumed that the space is filled with sand.

Today, the void in between the waste packages is not back-filled before the compartment is sealed. However, this is an option that can be accomplished at repository closure. In this analysis it is assumed that the void inside the compartments is left unfilled. A selection of geometrical data for the BMA vault is given in Table 4-3.

Table 4-3. Dimensions of the cavern, the concrete building and the storage compartments.

Property	Value	Reference
Vault		
Length [m]	160	Wiborgh and Lindgren, 1987
Width [m]	19.6	Wiborgh and Lindgren, 1987
Height [m]	16.5	Wiborgh and Lindgren, 1987
Excavated volume [m^3]	48 000	Wiborgh and Lindgren, 1987
Concrete building = sum of waste storage compartments		
Length, outer [m]	139.5	Calculated
Width, outer [m]	15.6	Calculated from data in SKB, 1993
Height, outer [m]	8.5	Calculated from data in SKB, 1993
Volume, outer [m^3]	18 520	Calculated
Volume, inner (total waste storage volume) [m^3]	14 400	Calculated
	14 000	Johansson, 1999
Thickness of concrete walls [m]	0.4[1]	Wiborgh and Lindgren, 1987
Thickness of concrete lid [m]	0.95	Riggare P, 2000a
Inner lid + concrete grout	0.45	Riggare P, 2000a
Outer reinforced lid	0.5	Riggare P, 2000a
Thickness of floor [m]	0.4	SKB, 1993
concrete	0.25	Forsgren, 1987
gravel	0.15	Forsgren, 1987
Large waste storage compartments		
Number of compartments	13	Wiborgh and Lindgren, 1987
Length, inner [m]	9.87	Wiborgh and Lindgren, 1987
Width, inner [m]	14.79	Wiborgh and Lindgren, 1987
Height, inner [m]	7.3	Wiborgh and Lindgren, 1987
Volume, inner [m^3]	1066	Calculated
Storage capacity, only moulds		
Number of concrete/steel moulds	576	Wiborgh and Lindgren, 1987
Storage capacity, moulds and drums		
Number of concrete/steel moulds	288	Wiborgh and Lindgren, 1987
Number of steel drums	1536	Wiborgh and Lindgren, 1987
Small waste storage compartments		
Number of compartments	2	Wiborgh and Lindgren, 1987
Length, inner [m]	4.95	Forsgren, 1987
Width, inner [m]	7.21	Forsgren, 1987
Height, inner [m]	7.3	SKB, 1993
Volume, inner [m^3]	260	Calculated

1) The wall facing the reloading zone is 0.6 m thick

The BMA vault is designed for 13 400 m3 of conditioned waste. The waste types are similar to those allocated to the Silo, e.g. ion-exchange resins and scrap and trash conditioned in cement or bitumen. About 55 % of the waste volume is ion-exchange resins and the remaining 45 % is scrap and trash. All of the waste is conditioned, about 76 % in cement and 24 % in bitumen.

The waste allocated to BMA is packed in concrete moulds, steel moulds and in steel drums with the same design and dimensions as those used for the Silo waste. Steel drums are placed on a steel plate or in a steel box with the same dimensions as the moulds before being loaded into the compartments in BMA.

There are also packages consisting of unconditioned scrap in a 100 l drum which is placed inside a 200 l drum with cement in between the two drums. In addition to the waste types specified above some 'Odd waste' will be allocated to BMA. Presently this waste is only defined in terms of metal content and quantity of cement used to stabilise the waste.

The waste allocated to BMA can be divided into the following categories:

- Concrete moulds with waste stabilised in cement.

- Steel moulds with waste stabilised in cement.

- Steel drums with waste stabilised in cement.

- Steel moulds with waste stabilised in bitumen.

- Steel drums with waste stabilised in bitumen.

About 54 % of the waste volume consist of concrete moulds, 27 % of steel moulds and 16 % of steel drums. The 'Odd waste' amounts to about 3 % of the waste volume. A compilation of different types of waste allocated to BMA is given in Table 4-4. The number of packages with steel components is based on the assumption that steel containers are used as packaging.

Table 4-4. Waste types allocated to BMA and the prognosticated number of waste packages and storage volume at repository closure (Riggare and Johansson, 2001).

Waste type		Package type	No of packages	Storage volume [m³]
O.01	Cement conditioned ion-exchange resins	Concrete mould (0.1 m) [1]	715	1235
O.23	Trash in cement	Concrete mould (0.1 m) [1]	696	1203
C.01	Cement conditioned ion-exchange resins	Concrete mould (0.1 m) [1]	23	40
C.23	Trash in cement	Concrete mould (0.1 m) [1]	88	152
R.01	Cement conditioned ion-exchange resins	Concrete mould (0.1 m) [1]	1702	2941
R.10	Cement conditioned sludge	Concrete mould (0.1 m) [1]	136	235
R.15	Cement conditioned ion-exchange resins	Steel container	295	510
R.23/steel	Trash in cement	Steel container	486	840
R.23/concrete	Trash in cement	Concrete mould (0.1 m) [1]	343	593
B.05	Bitumen conditioned ion-exchange resins	Steel drum	4230	1037
F.05	Bitumen conditioned ion-exchange resins	Steel drum	1718	421
F.15	Cement conditioned ion-exchange resins	Steel container	11	19
F.17	Bitumen conditioned ion-exchange resins	Steel container	879	1519
F.23/steel	Non-solidified trash	Steel container	270	467
F.23/concrete	Trash in cement	Concrete mould (0.1 m) [1]	54	93
S.09	Cement conditioned sludge	Steel drum	382	94
S.21	Unconditioned scrap	Steel drum in steel drum with cement in between	1493	366
S.23	Trash in cement	Concrete mould (0.1 m) [1]	61	105
Other waste	Steel components	Unknown	238 [2]	411
Total			13820	12281

1) 0.1 m refers to the thickness of the mould walls.
2) Based on the assumption of steel container as packaging

BTF

The rock vaults for concrete tanks, 1BTF and 2BTF, consists of two identical rock vaults, 160 m long with a wall height of 6.5 m, a maximum height of 9.5 m and a width of 14.7 m. The bottom of the vaults is covered by a 0.3 m thick layer of gravel and a 0.4 m thick concrete floor on top of the gravel. The amount of construction concrete in the floor is estimated to be 1350 m³ /Wiborgh and Lindgren, 1987/. The walls and ceiling of the vaults are covered by shotcrete, in total about 250 m³ per vault /Wiborgh and Lindgren, 1987/.

In one of the vaults, 2BTF, only concrete tanks are placed. The other vault, 1BTF, contains both concrete tanks and steel drums and also steel containers and some concrete moulds. The waste in the concrete tanks is de-watered, low-level ion exchange resin and the steel drums contain ashes. The steel containers contain graphite and the concrete moulds low-level ion-exchange resins that are stabilised in cement.

In the vault 1BTF, concrete tanks are stacked two high around the walls of the vault. Concrete moulds are used to make "compartments" where drums with ashes can be stacked. The drums are piled in 10 layers with alternating 19 and 18 drums in each layer in the row. To make a separating "wall" the moulds are stacked four moulds high and nine moulds wide. A total of six compartments are needed to make room for 6 479 steel drums. Five of the compartments will be completely filled, containing 1 110 drums each, and the last compartment will hold 929 drums. When a compartment is filled with drums, it is sealed using concrete grout. In order to prevent concrete from pouring out between the concrete tanks and moulds, the inside of the "compartment" walls is covered by geotextile. The rest of the vault is used for concrete tanks, steel boxes and odd waste.

At repository closure of 1BTF, 0.4 m thick prefabricated concrete lids will be placed on top of the concrete tanks. Concrete is then used to fill the space between the rock walls and the waste packages in the whole vault up to a height of 5.4 m. The space between the concrete tanks in the part of the vault used for concrete tanks is also filled with concrete to the same height. On top of the cement a 0.4 m thick reinforced slate of concrete will be cast and the remaining volume is back-filled using sand.

In 2BTF, the concrete tanks are stacked in rows of four tanks side by side and two tanks high. At repository closure, prefabricated concrete lids will be placed on top of the concrete tanks in 2BTF in the same way as in 1BTF. The vault will be sealed with concrete and sand in the same way as 1BTF. Geometrical data for the BTF vaults are compiled in Table 4-5.

Table 4-5. Dimensions of the BTF caverns and the waste storage area

Property	Value	Reference
1BTF and 2BTF		
Length [m/vault]]	160	Wiborgh and Lindgren, 1987
Width [m/vault]	14.7	Wiborgh and Lindgren, 1987
Height [m/vault]	9.5	Wiborgh and Lindgren, 1987
Excavated volume [m^3/vault]	20 000	Wiborgh and Lindgren, 1987
Length of waste storage area [m/vault]	138	Wiborgh and Lindgren, 1987
Width of waste storage area [m/vault]	13.9	Riggare, 2000b
Height of waste storage area [m/vault]	5.4	Riggare, 2000b
Storage capacity [m^3/vault]	7900	Wiborgh and Lindgren, 1987
	7800	Johansson, 1999
Storage capacity [number of concrete tanks/vault]	790	Wiborgh and Lindgren, 1987
	780	Calculated from data in Johansson, 1999
1BTF – "compartments"		
Number of drums in each layer in one row	19/18	Site observation
Number of drums in all 10 layers in one row	185	Calculated
Total number of drums in one "compartment"	1110	Calculated
Inner length of one "compartment" [m]	5.4	Calculated from drum dimensions
Inner width of one "compartment" [m]	11.3	Calculated
Inner volume of one "compartment" [m3]	329.5	Calculated

The two vaults, 1BTF and 2BTF, are designed for about 10 000 m^3 of waste each. The effective volume of the vaults is about 20 000 m^3. In 1BTF the waste is comprised of ion exchange resins (27 %), ashes (20 %), graphite (1 %), sludge (0.5 %), trash (less than 0.2 %) and steel waste (52 %), and in 2BTF the waste consists of ion exchange

resins. Most of the resins in 1BTF are non-solidified, 85 %, but there are also conditioned resins. The ashes, the sludge and the trash are conditioned with cement, while the graphite and the steel waste are unconditioned. In 2BTF all the waste is non-solidified.

The waste allocated to 1BTF is packed in concrete tanks, steel drums in steel drums, steel boxes and concrete moulds. In 2BTF only concrete tanks are used. The dimensions of the concrete moulds are the same as the concrete moulds used in the Silo and BMA. The concrete tanks are 3.3 m long, 1.3 m wide and 2.3 m high and the steel drums are a 100 l drum placed in a 200 l drum with concrete between. The outer drum has a diameter of about 0.6 m and a height of about 0.9 m. The steel boxes are 1.2 m long and 0.8 m wide and high.

The waste allocated to 1BTF can be divided into the following categories:

- Concrete tanks with non-solidified resins.

- Steel drum in steel drum with cement between, containing ashes.

- Steel box 1.2x0.8x0.8 m, containing unconditioned graphite ("Berglöfs").

- Concrete mould with waste stabilised in cement.

In addition to the waste types specified above 'Odd waste' will be allocated to 1BTF. This waste is only defined in terms of metal content. About 22 % of the waste volume in 1BTF consist of concrete tanks, 25 % of steel drums, less than 0.1 % of steel boxes and 4 % of concrete moulds. The 'Odd waste' amounts to about 49 % of the waste volume.

The waste allocated to 2BTF is of one category: concrete tanks with non-solidified resins.

BLA

The rock vault for low level waste, BLA, is 160 m long, 14.7 m wide, has a wall height of 9 m and a maximum height of 12.5 m. The waste is piled to 7.8 m height and the bottom of the vault is covered by a 0.3 m thick layer of gravel. On top of the gravel a concrete floor, 0.4 m thick, is placed.

The amount of construction concrete in the floor is estimated to be 800 m^3 /Wiborgh and Lindgren, 1987/. The walls and ceiling of the cavern are covered by shotcrete, in total about 300 m^3 /Wiborgh and Lindgren, 1987/. The waste is packed in steel containers (ISO 10' or 20') that are piled on a concrete floor in the vault, two in a row and three full-height containers on top of each other. There are presently no plans for any backfill in the BLA vault. Some geometrical data for the BLA vault are compiled in Table 4-6.

BLA is designed for approximately 12 000 m^3 of unconditioned and bitumenised waste. Most of the waste is non-solidified trash, about 87 %, 4 % is bitumenised ion-exchange resins and 9 % odd waste.

Table 4-6. Dimensions of the BLA cavern and the waste storage area

Property	Value	Reference
Length [m]	160	Wiborgh and Lindgren, 1987
Width [m]	14.7	Wiborgh and Lindgren, 1987
Height [m]	12.7	Wiborgh and Lindgren, 1987
Excavated volume [m^3]	27 000	Wiborgh and Lindgren, 1987
Length of waste storage area [m]	127	Wiborgh and Lindgren, 1987
	160	Calculated from waste storage volume given in Johansson, 1999
Width of waste storage area [m]	12.1	Corresponds to the length of 2 20' ISO containers (2 x 6.058 m)
Height of waste storage area [m]	7.8	Corresponds to the height of 3 full-height ISO containers (3 x 2.591 m)
Storage capacity [m^3]	11 500	Wiborgh and Lindgren, 1987
	15 100	Johansson, 1999
Storage capacity [number of containers][1]	300	Wiborgh and Lindgren, 1987

1) Full-height 20' containers

The waste allocated to BLA can be divided into the following categories:

- ISO-containers with non-solidified trash.

- Steel drums with bitumenised ion-exchange resins.

- Steel drums with non-solidified trash in steel drum placed in an ISO-container.

In addition to the waste types specified above some 'Odd waste' will be allocated to BLA. Presently this waste is only defined in terms of metal content and it is assumed to have the same dimensions as an ISO-container.

About 76 % of the waste volume consist of ISO-containers, 4 % of steel drums in ISO-containers and 11 % of steel drums in steel drums placed in ISO-containers. About 9 % of the waste volume is odd waste. An overview of the different types of waste and the number of waste packages that are allocated to BLA is given in Table 4-7. The number of waste packages is based on the assumption that the ISO containers all are half height.

The waste allocated to BLA is packed in ISO-containers, steel drums in ISO-containers and steel drums in steel drums placed in ISO-containers. There are ISO-containers of different sizes, but here all ISO-containers are assumed to be 6 m long, 2.5 m wide and 1.3 m high (half height). The drums have a diameter of about 0.6 m and a height of about 0.9 m.

Table 4-7. Waste types allocated to BLA and the prognosticated number of waste packages and storage volume at repository closure /Riggare and Johansson, 2001/.

Waste type		Package type	No of packages[1]	Storage volume [m^3]
O.12	Scrap and trash	ISO container	80	1600
R.12	Scrap and trash	ISO container	103	2060
B.12	Scrap and trash	ISO container	272	5440
B.20	Ion-exchange resins, stabilised in bitumen	36 steel drums in an ISO container	12	240
F.12	Scrap and trash	ISO container	28	560
F.20	Ion-exchange resins, stabilised in bitumen	36 steel drums in ISO container	15	300
S.12	Scrap and trash	ISO container	31	620
S.14	Scrap and trash	36 steel drums (200 l) with inner steel drums (100 l) placed in an ISO container [2]	73	1460
Total			614	12 280

1) Expressed as half-height, 20' ISO containers
2) the space between the inner and outer drum is filled with cement

4.2.2 Dimensions selected in the analysis

Data on repository dimensions given in the previous section are used for calculating volumes, areas etc, to be used as input data in different calculation models. The raw data given in the previous sections can be interpreted in different ways depending on what it will be used for. What is conservative for one model may not be conservative for another model. Data selected for the migration models can be found in appendices in Lindgren *et al.* /2001/. Data used for the hydrology modelling and the modelling of gas influenced release of radionuclides are given in Holmén and Stigsson /2001a/ and Moreno *et al.* /2001/, respectively.

4.3 Construction materials and waste composition

The cementitious materials that can be found in the SFR repository are mainly: structural concrete in buildings and waste packaging, concrete grout used as backfill around the waste packages in the Silo, BMA and BTF vaults and cement mortar and grout used as conditioning material for the waste. The mixing proportions for the different concrete types in SFR are given in Table 4-8. Data on structural concrete and Silo grout are from Höglund /2001/ and data on BTF grout from Riggare /2000a/.

A mixture consisting of 90 % sand and 10 % bentonite by weight is used as backfill in the bottom of the Silo repository. A layer of the same mixture will also be added in the upper part of the Silo repository at repository closure.

Sand and/or gravel will be used as backfill in the Silo and the vaults at repository closure.

The wastes comprise of different materials and are packed in different types of packaging. A detailed description of waste characteristics with respect to material composition and quantities are given in Riggare and Johansson /2001/.

Table 4-8. Mixing proportions for concrete in SFR [kg/m^3]

Component	Structural concrete	Silo grout	1BTF grout	
			Bottom[1]	Top[2]
Cement	350	325	340	265
Water	164.5	366	252[3]	141
Ballast	1829	1302	1630	1890
w/c ratio	0.47 (0.46 – 0.49)	1.125	0.74	0.53 (0.75)[4]

1) up to half the height of the uppermost layer of steel drums
2) from half of the height of the uppermost layer of steel drums
3) calculated from reported w/c ratio and cement content
4) value including specified maximum humidity in ballast material

4.4 Radionuclide inventory

4.4.1 Data needed

For the radionuclide migration calculations it is required that the radionuclide inventory is specified for each repository part and for the different waste categories.

4.4.2 Data Sources and evaluation of uncertainties

An updated estimate of the inventory of radionuclides in SFR-1 at repository closure has been made /Riggare and Johansson, 2001/. The sources used for this estimate are:

- a database for waste that are already deposited in SFR-1 /TRIUMF, 2000/

- a database for gamma emitting nuclides in waste from Studsvik or their waste type descriptions

- a database over transuranic elements in Swedish reactors

- correlation factors derived for the preliminary assessment of a deep repository for long-lived low- and intermediate- level waste /SKB, 1999b/

- a prognosis of the number of waste packages of each waste category in SFR-1 at repository closure

- nuclide half-life /Firestone, 1998/

The method used for estimating the nuclide inventory, described in detail in Riggare and Johansson /2001/, is considered to give a realistic estimate of the inventory. The result of the estimate is an inventory for SFR-1 of in total $1.0 \cdot 10^{15}$ Bq by the end of 2030.

The updated realistic estimate of the inventory will not be used in the migration calculations. There are at least two reasons for this:

- The realistic inventory is still an estimate. Uncertainties in future inventories would be easily treated by instead analysing an upper bound.

- The final inventory is still a matter of decision. For example, waste originally planned for SFL 3-5 could go to SFR and vice versa. Consequently, it is better to analyse the safety for a designed upper target inventory. If the repository is shown to be safe for this inventory any actual inventory below this number will also be safe. This is also the rationale behind the present license, which allows an upper limit of 10^{16} Bq to be disposed.

The simplest option would be to use the inventory used in the past analyses. There are, however, some problems that needs to be resolved:

- The old inventory lacks some of the important nuclides (like Cl-36)

- The distribution of inventory to different waste form affects the result.

In order to resolve this problem a conservative estimate of the inventory has been selected for the analysis. How this conservative inventory is derived is described in Riggare and Johansson /2001/.

4.4.3 Selected radionuclide inventory

The estimated radionuclide inventory in SFR-1 at repository closure /Riggare and Johansson, 2001/ includes 59 radionuclides. However, not all of them are expected to be important for the evaluation of the safety after closure of the repository. A first screening of nuclides has been made based on a scenario in which dose to man is obtained by drinking well water. The worst case would be if the whole nuclide inventory were released to a well immediately after repository closure. However, it is reasonable to assume that it takes at least three generations, or about 100 years, before knowledge of a repository can be considered to be lost /Morén *et al.,* 1998/. Consequently, it is unlikely that a well will be sunk in the repository area earlier than year 2130.

A scenario in which nuclides are released to a well in year 2130 is assumed and the nuclide concentration in the well water is based on the following premises:

- the well has a capacity equal to 30 % of the excavated volume within the Silo

- the amount of nuclides released to the well corresponds to the initial inventory within the Silo taking 100 years of decay into account

- radionuclide sorption is not accounted for.

The screening is based on the radionuclide inventory in the Silo since it is the repository part containing the highest activity content. If the analysis were based on any of the other repository parts, additional nuclides could be excluded. It has been checked that all nuclides excluded based on the Silo inventory would also be excluded for the other repository parts. In addition, estimates of an early release of all radionuclides from BLA to Öregrundsgrepen do not imply that other radionuclides must be considered in the analysis.

The nuclide concentration in the well is transformed into a dose rate using factors for committed effective dose from ingestion of radionuclides by an adult /EU, 1996/ and assuming that an individual consumes 600 litres of water annually. An annual dose less than 0.01 mSv/year is used as a screening criteria and 19 radionuclides were found to give dose rates below this value. Even though ^{3}H and ^{107}Pd gave dose rates below the limit it was decided to include them in the final set of radionuclides. The inventory of the excluded radionuclides (^{10}Be, ^{55}Fe, ^{106}RU, ^{107}Pd, ^{125}Sb ^{134}Cs, ^{133}Ba, ^{147}Pm, ^{155}Eu, ^{210}Pb, ^{226}Ra, ^{227}Ac, ^{229}TH, ^{230}Th, ^{232}Th, ^{231}Pa, ^{233}U) can be found in Riggare and Johansson /2001/. The radionuclides included in the assessment are reduced from 59 to 42 and the inventory at repository closure is compiled in Table 4-9.

Table 4-9. Radionuclide inventory (Bq) in SFR-1 at repository closure (year 2030) /Riggare and Johansson, 2001/.

Nuclide	Half-life [years] [a]	Silo	BMA	1BTF	2BTF	BLA
^{3}H	12.3	$5.8 \cdot 10^{11}$	$3.3 \cdot 10^{10}$	$3.3 \cdot 10^{9}$	$5.3 \cdot 10^{9}$	$6.6 \cdot 10^{8}$
^{14}C inorg	5730	$2.0 \cdot 10^{13}$	$1.9 \cdot 10^{12}$	$2.3 \cdot 10^{12}$	$2.7 \cdot 10^{11}$	$3.9 \cdot 10^{10}$
^{14}C org	5730	$1.8 \cdot 10^{12}$	$1.7 \cdot 10^{11}$	$1.8 \cdot 10^{11}$	$3.0 \cdot 10^{10}$	$3.3 \cdot 10^{7}$
^{36}Cl	301 000	$4.7 \cdot 10^{10}$	$3.4 \cdot 10^{9}$	$3.0 \cdot 10^{8}$	$5.4 \cdot 10^{8}$	$8.2 \cdot 10^{7}$
^{60}Co	5.27	$1.8 \cdot 10^{15}$	$7.1 \cdot 10^{13}$	$5.4 \cdot 10^{12}$	$9.1 \cdot 10^{12}$	$1.0 \cdot 10^{12}$
^{59}Ni	76 000	$2.1 \cdot 10^{13}$	$2.1 \cdot 10^{12}$	$1.8 \cdot 10^{11}$	$3.0 \cdot 10^{11}$	$3.9 \cdot 10^{10}$
^{63}Ni	100.1	$3.6 \cdot 10^{15}$	$3.2 \cdot 10^{14}$	$2.9 \cdot 10^{13}$	$4.7 \cdot 10^{13}$	$6.2 \cdot 10^{12}$
^{79}Se	1 130 000	$1.9 \cdot 10^{10}$	$1.4 \cdot 10^{9}$	$1.2 \cdot 10^{8}$	$2.2 \cdot 10^{8}$	$3.3 \cdot 10^{7}$
^{90}Sr	28.8	$2.4 \cdot 10^{14}$	$1.4 \cdot 10^{13}$	$1.3 \cdot 10^{12}$	$2.3 \cdot 10^{12}$	$3.6 \cdot 10^{11}$
^{93}Zr	1 530 000	$2.1 \cdot 10^{10}$	$2.1 \cdot 10^{9}$	$1.8 \cdot 10^{8}$	$3.0 \cdot 10^{8}$	$3.9 \cdot 10^{7}$
^{93m}Nb	16.1	$7.6 \cdot 10^{12}$	$4.9 \cdot 10^{11}$	$4.7 \cdot 10^{10}$	$7.6 \cdot 10^{10}$	$9.7 \cdot 10^{9}$
^{94}Nb	20 300	$2.1 \cdot 10^{11}$	$2.1 \cdot 10^{10}$	$1.8 \cdot 10^{9}$	$3.0 \cdot 10^{9}$	$3.9 \cdot 10^{8}$
^{93}Mo	4000	$1.1 \cdot 10^{11}$	$1.0 \cdot 10^{10}$	$9.1 \cdot 10^{8}$	$1.5 \cdot 10^{9}$	$1.9 \cdot 10^{8}$
^{99}Tc	211 000	$2.4 \cdot 10^{13}$	$1.7 \cdot 10^{12}$	$1.5 \cdot 10^{11}$	$2.7 \cdot 10^{11}$	$4.1 \cdot 10^{10}$
^{107}Pd	6 500 000	$4.7 \cdot 10^{9}$	$3.4 \cdot 10^{8}$	$3.0 \cdot 10^{7}$	$5.4 \cdot 10^{7}$	$8.2 \cdot 10^{6}$
^{108m}Ag	418	$1.2 \cdot 10^{12}$	$1.2 \cdot 10^{11}$	$1.0 \cdot 10^{10}$	$1.7 \cdot 10^{10}$	$2.2 \cdot 10^{9}$
^{113m}Cd	14.1	$8.2 \cdot 10^{11}$	$3.6 \cdot 10^{10}$	$3.6 \cdot 10^{9}$	$6.4 \cdot 10^{9}$	$1.0 \cdot 10^{9}$
^{126}Sn	100 000	$2.4 \cdot 10^{9}$	$1.7 \cdot 10^{8}$	$1.5 \cdot 10^{7}$	$2.7 \cdot 10^{7}$	$4.1 \cdot 10^{6}$
^{129}I	$1.6 \cdot 10^{7}$	$1.4 \cdot 10^{9}$	$1.0 \cdot 10^{8}$	$9.1 \cdot 10^{6}$	$1.6 \cdot 10^{7}$	$2.5 \cdot 10^{6}$
^{135}Cs	2 300 000	$2.4 \cdot 10^{10}$	$1.7 \cdot 10^{9}$	$1.5 \cdot 10^{8}$	$2.7 \cdot 10^{8}$	$4.1 \cdot 10^{7}$
^{137}Cs	30.1	$2.5 \cdot 10^{15}$	$1.4 \cdot 10^{14}$	$1.4 \cdot 10^{13}$	$2.4 \cdot 10^{13}$	$3.7 \cdot 10^{12}$
^{151}Sm	90	$1.1 \cdot 10^{13}$	$7.5 \cdot 10^{11}$	$6.9 \cdot 10^{10}$	$1.2 \cdot 10^{11}$	$1.9 \cdot 10^{10}$
^{152}Eu	13.5	$9.2 \cdot 10^{10}$	$4.0 \cdot 10^{9}$	$4.4 \cdot 10^{11}$	$7.1 \cdot 10^{8}$	$1.1 \cdot 10^{8}$
^{154}Eu	8.59	$7.9 \cdot 10^{13}$	$2.7 \cdot 10^{12}$	$2.8 \cdot 10^{11}$	$4.8 \cdot 10^{11}$	$7.6 \cdot 10^{10}$
^{166m}Ho	1200	$8.4 \cdot 10^{10}$	$8.2 \cdot 10^{9}$	$7.2 \cdot 10^{8}$	$1.2 \cdot 10^{9}$	$1.5 \cdot 10^{8}$
^{232}U	68.9	$2.0 \cdot 10^{7}$	$1.1 \cdot 10^{6}$	$8.1 \cdot 10^{4}$	$6.3 \cdot 10^{4}$	$6.1 \cdot 10^{4}$
^{234}U	246 000	$8.4 \cdot 10^{8}$	$4.5 \cdot 10^{7}$	$3.5 \cdot 10^{6}$	$2.7 \cdot 10^{6}$	$2.5 \cdot 10^{6}$
^{235}U	$7.0 \cdot 10^{8}$	$1.7 \cdot 10^{7}$	$8.9 \cdot 10^{5}$	$7.1 \cdot 10^{4}$	$5.4 \cdot 10^{4}$	$5.1 \cdot 10^{4}$
^{236}U	$2.3 \cdot 10^{7}$	$2.5 \cdot 10^{8}$	$1.3 \cdot 10^{7}$	$1.1 \cdot 10^{6}$	$8.2 \cdot 10^{5}$	$7.6 \cdot 10^{5}$
^{238}U	$4.5 \cdot 10^{9}$	$3.3 \cdot 10^{8}$	$1.8 \cdot 10^{7}$	$1.4 \cdot 10^{6}$	$1.1 \cdot 10^{6}$	$1.0 \cdot 10^{6}$
^{237}Np	2 140 000	$3.3 \cdot 10^{8}$	$1.8 \cdot 10^{7}$	$1.4 \cdot 10^{6}$	$1.1 \cdot 10^{6}$	$1.0 \cdot 10^{6}$
^{238}Pu	87.7	$2.8 \cdot 10^{12}$	$1.5 \cdot 10^{11}$	$1.1 \cdot 10^{10}$	$8.9 \cdot 10^{9}$	$8.5 \cdot 10^{9}$
^{239}Pu	24 100	$2.8 \cdot 10^{11}$	$1.5 \cdot 10^{10}$	$1.2 \cdot 10^{9}$	$9.1 \cdot 10^{8}$	$8.5 \cdot 10^{8}$
^{240}Pu	6560	$5.6 \cdot 10^{11}$	$3.0 \cdot 10^{10}$	$2.4 \cdot 10^{9}$	$1.8 \cdot 10^{9}$	$1.7 \cdot 10^{9}$
^{241}Pu	14.4	$3.1 \cdot 10^{13}$	$1.6 \cdot 10^{12}$	$1.0 \cdot 10^{11}$	$8.2 \cdot 10^{10}$	$8.8 \cdot 10^{10}$
^{242}Pu	373 000	$2.5 \cdot 10^{9}$	$1.3 \cdot 10^{8}$	$1.1 \cdot 10^{7}$	$8.2 \cdot 10^{6}$	$7.6 \cdot 10^{6}$
^{241}Am	432	$6.1 \cdot 10^{12}$	$4.3 \cdot 10^{10}$	$3.4 \cdot 10^{9}$	$2.6 \cdot 10^{9}$	$2.5 \cdot 10^{9}$
^{242m}Am	141	$7.5 \cdot 10^{9}$	$4.0 \cdot 10^{8}$	$3.1 \cdot 10^{7}$	$2.4 \cdot 10^{7}$	$2.3 \cdot 10^{7}$
^{243}Am	7370	$2.5 \cdot 10^{10}$	$1.3 \cdot 10^{9}$	$1.1 \cdot 10^{8}$	$8.1 \cdot 10^{7}$	$7.6 \cdot 10^{7}$
^{243}Cm	29.1	$1.0 \cdot 10^{10}$	$5.3 \cdot 10^{8}$	$3.8 \cdot 10^{7}$	$3.0 \cdot 10^{7}$	$3.0 \cdot 10^{7}$
^{244}Cm	18.1	$1.1 \cdot 10^{12}$	$5.9 \cdot 10^{10}$	$3.9 \cdot 10^{9}$	$3.1 \cdot 10^{9}$	$3.3 \cdot 10^{9}$
^{245}Cm	8500	$2.5 \cdot 10^{8}$	$1.3 \cdot 10^{7}$	$1.1 \cdot 10^{6}$	$8.1 \cdot 10^{5}$	$7.6 \cdot 10^{5}$
^{246}Cm	4730	$6.7 \cdot 10^{7}$	$3.6 \cdot 10^{6}$	$2.8 \cdot 10^{5}$	$2.2 \cdot 10^{5}$	$2.0 \cdot 10^{5}$

a) Firestone /1998/

5 Water flow in engineered barriers

In this chapter, the hydrogeological data used in the calculation of radionuclide migration in the repository vaults are described.

5.1 Data needed and data sources

As indicated in Section 3.2, the near-field migration model requires input in terms of size and direction of water flow in the repository vaults as well as the Darcy velocity (groundwater flux) in the rock surrounding the repository vaults. Data are required both for the case with engineered barriers that are intact and for the case with fractured/degraded barriers. These data are derived from the results of the modelling with the detailed hydrogeology model /Holmén and Stigsson, 2001a/ and the results are compiled in a large number of tables in a separate document /Holmén and Stigsson, 2001b/.

For the case with intact barriers, the water flow in the repository vaults are calculated assuming a hydraulic conductivity of structural concrete of $8.3 \cdot 10^{-10}$ m/s. This conductivity is chosen as representative for structural concrete with some small penetrating fractures. A 10 times higher conductivity is used for the concrete grout surrounding the waste packages in the Silo and BTF vaults and a conductivity of 10^{-5} m/s is assumed for the rock fill in the vaults. The sand/bentonite barriers in the bottom and the top of the Silo are assigned a conductivity of $1 \cdot 10^{-9}$ m/s and the bentonite surrounding the walls of the Silo is assigned an average conductivity of $6 \cdot 10^{-12}$ m/s. From these values, the hydraulic conductivity of the different structures included in the detailed hydrological model is calculated (see Holmén and Stigsson /2001a/).

For the case with degraded barriers, a higher conductivity of the different barriers is assumed. All concrete and bentonite barriers in the Silo is assigned a conductivity of 10^{-8} m/s. For the BMA and BTF vaults the conductivity of the degraded section is set to 10^{-5} m/s /Holmén and Stigsson, 2001a/.

5.2 Derivation of data

The groundwater flow, calculated with the detailed hydrology model, corresponds to a situation when the repository is closed and the repository vaults are no longer kept dry, but filled with groundwater. Under such conditions the vault receives water from the rock mass at different sections along the vault and gives water to the rock mass at other sections along the vault. Thus, the flow and velocity of water inside the vault varies along the vault. The flow of water in the vault can be studied based on different concepts, e.g. "specific flow", "total flow" and "net flow". The detailed flow values derived from the hydrogeological modelling and used as input to the migration model are primarily given as net flows. The net flow is defined based on a mass balance taken over a studied area.

To derive the input data to the migration model, the repository vaults are divided into different sections. Each section contains several parallelepipeds (blocks) as given by the finite difference cells of the hydrogeological model and these blocks are the volumes studied. Each block has six faces (even if it contains several finite difference cells) and these faces are the areas for which the net flow is calculated. The separation of the finite difference cells into different sections and blocks was done to produce details of flow

that fitted the layout of the near-field migration model. Details regarding the separation of the finite difference cells of the hydrogeological flow model into blocks that fitted the migration model are given in Holmén and Stigsson /2001b/.

The repository vaults BMA, BLA and BTF are divided into five sections in the horizontal direction that represent the part of the tunnels where the waste is stored and two sections representing the loading areas at each end of the vault. Each section that contains waste is then divided into a waste domain block (encapsulation-block) and four blocks that represents the volumes that surrounds the waste domain. For the encapsulation-block, the net flow is given for its six faces. The net flow is also given for the blocks that surrounds the encapsulation in terms of six values of net flow for the block:

- above the encapsulation-block

- below the encapsulation-block

- to the left of the encapsulation-block and

- to the right of the encapsulation-block.

Hence, for each of the studied repository vaults there will be 150 values of net flow for the 5 sections that represents the waste domain and surrounding flow-barriers and 12 values of net flow for the loading areas for each time period studied.

The Silo is divided into a total of eight vertical sections of which five represent the waste inside the encapsulation. The remaining three represent the sand/bentonite at the base of the encapsulation, the sand/bentonite at the top of the encapsulation and the top fill above the sand/bentonite. Each section that contains waste is further divided into an encapsulation-block (waste domain) and one block that represents the horizontally surrounding bentonite barrier. The remaining three sections are considered as one block each. For all these blocks the flow is given as the axial and radial net flows, which produces 48 values of flow for each time period studied.

Due to the progressive land rise and shore line displacement, the water flow in the repository vaults will change with time. In the migration model this is simulated by stepwise changes in the flow values. For that purpose, flow values was calculated for seven different time periods: 2000 AD, 3000 AD, 4000 AD, 5000 AD, 6000 AD and 7000 AD.

Also the average specific flow (Darcy velocity) at a distance of approximately 5 metres from the repository vaults and into the surrounding rock mass is derived from the hydrogeological modelling results. Such flow values are given for each section and time period studied.

5.3   Derived data

As indicated above, a large number of flow values are derived and used as input to the migration modelling. All these data are tabulated in a separate document /Holmén and Stigsson, 2001b/ and therefore not repeated here.

5.4   Data uncertainties

Theoretically the derivation of input data in terms of a net flow may underestimate the total flow through the surface if there is both discharge and recharge on the face, but in reality flow directions are quite uniform and this consideration has little practical

impact. Instead, the largest uncertainty is probably associated with the permeability (hydraulic conductivity) selected for the different materials and the changes in these entities with time. However, the values on conductivity for concrete and bentonite barriers are selected in order not to under estimate their permeability, both in the case with intact barriers and in the case with degraded barriers. The selected conductivity of the rock fill in the repository vaults may, on the other hand, be lower than would be expected. However, a higher conductivity of the rock fill will further reduce the water flow through the waste storage area in BMA and the BTF vaults since this means a higher contrast in conductivity between waste storage area and the rock fill outside /Holmén and Stigsson, 2001a/. Furthermore, the use of a lower conductivity of the rock fill could implicitly simulate a potential future decrease in porosity due to chemical alteration of the rock fill by concrete pore water.

6 Chemical and physical data – engineered barriers

In this chapter, the different chemical and physical data needed as input to the migration model are discussed and compiled. These data are radionuclide solubility, sorption and diffusivity and porosity and density of the different materials.

6.1 Solubility

6.1.1 Data needed

Sorption is expected to be the major process that affects the concentration of radionuclides in the barriers in the repository vaults in SFR. However, some elements may have such a low solubility that even if sorption is accounted for, the concentration in the pore water in the barriers will be determined by the solubility. Because of the relatively small amounts of radionuclides in the waste and quite large amounts of concrete and cement in the different repository parts, sorption rather than solubility is expected to determine the source term release. The BLA vault does not contain any concrete barriers, but instead the dilution volume is larger than in the other vaults and the concentration of radionuclides in the waste is lower.

6.1.2 Source of data

The solubility of elements is dependent on the water chemistry and important parameters are pH, redox conditions and the presence of complexing agents. In this respect, the conditions in the Silo and in the BMA and BTF vaults are very similar to the conditions in the near-field barriers of the SFL 3-5 repository. The solubility of different elements that was used in the preliminary safety assessment of SFL 3-5 /SKB, 1999b/ should therefore also be applicable for the safety assessment of SFR.

6.1.3 Selected data

As indicated above, the solubility may be of importance for a few elements only. The basic approach suggested is therefore to neglect any potential limits in solubility and instead assume that the total inventory of radionuclides is dissolved in the water in the waste packages. This is in accordance with the assumptions made in the previous safety assessments of SFR-1 /SKB, 1987 and 1991/.

If it develops a need of displaying the effect of limited solubility of certain elements it is suggested to use the solubility limits derived for the preliminary safety assessment of the SFL 3-5 repository. These data are given in Table 6-1 in case of no impact of complexing agents on the solubility limits /Skagius et al., 1999/. If complexing agents are present no solubility limits should be accounted for /Skagius et al., 1999/.

Table 6-1. Solubility limits in concrete pore water, pH > 10, reducing conditions and no impact of complexing agents /Skagius et al., 1999/

Ox. state	Element	Solubility (M)
M(II)	Be, Cd	10^{-3}
	Fe, Co	10^{-5}
	Ni	10^{-7}
	Pb	10^{-6}
M(III)	Am, Cm, Pm	$9 \cdot 10^{-8}$
M(IV)	Tc	10^{-7}
	Zr	10^{-4}
	Th, Pa, U, Np, Pu	$5 \cdot 10^{-9}$
M(V)	Nb	10^{-6}

6.1.4   Uncertainties

According to Skagius *et al*. /1999/ the solubility limits recommended for the safety assessment of SFL 3-5 are based on literature data in the whole alkaline range at pH > 10. A pessimistic approach was used by selecting the highest of the values reported in the literature for this pH range.

6.2   Sorption

6.2.1   Data needed

To calculate the near-field release of radionuclides sorption data for the near-field barriers are required. The near-field barriers that are considered as sorption barriers in the different repository parts are cement/concrete and rock fill in the BMA and BTF vaults and cement/concrete, bentonite and sand/bentonite in the Silo. No sorption barriers are considered for the BLA vault.

Different metals are present in the waste to SFR. With time these metals will corrode and the corrosion products that are formed in largest quantity are different oxides/hydroxides of iron. Such compounds are well known to adsorb and co-precipitate other metal ions present in solution. For example, Savage *et al.,* /2000/ suggest sorption data that are based on experimental results reported in the literature. However, there are still uncertainties associated with the quantification of sorption on corrosion products and furthermore, the effect might not be so important in relation to sorption on concrete in the repository parts where large quantities of concrete is present. It is therefore suggested that the potential effects of sorption and co-precipitation with corrosion products is discussed in the safety assessment, but not considered in the quantitative assessment of radionuclide release.

Sorption in the near-field barriers is dependent on the water composition in the barriers. Based on a compilation of data on the present composition of the groundwater in the Forsmark area a groundwater composition for the time period when SFR is located beneath the seabed (salt-water period) is proposed /Höglund, 2001/. This water has a pH of 7.3, is reducing and saline with a chloride concentration of 5 g/l. Because the groundwater is saline at repository closure and will prevail saline for at least a thousand year and because the pore water in both concrete and bentonite barriers initially will have a high ionic strength, sorption data for saline water conditions are selected. This means that the suggested sorption data are lower than they would be in non-saline water for elements that have a sorptivity that is dependent on the salinity of the water.

In regard to sorption in bentonite, the use of data from batch experiments to estimate the retention in bentonite barriers is questionable, e.g. due to differences in water to solid ratio. On the other hand, it is also difficult to determine sorption data from transient diffusion experiments since diffusion and sorption is coupled processes and uncertainties in the effective diffusivity in the sample will affect the result. The ideal situation would be to be able to use the same model in the evaluation of experimental data as is used in the migration modelling in a safety assessment. In addition it would be beneficial if the input to the migration model would be in terms of an apparent and an effective diffusivity instead of a K_d-value and an effective diffusivity from which the model calculates an apparent diffusivity. This ideal situation is not prevailing here and therefore the selection of input data has to be made in terms of K_d-values and effective diffusivities based on data reported in the literature.

6.2.2 Source of data

Cement/concrete

Due to the expected similarity in composition of the pore water in the concrete barriers in SFR and the concrete barriers in an SFL 3-5 repository, the sorption data selected for sorption in the concrete barriers in SFR are the same as those used in the preliminary safety assessment of the SFL 3-5 repository /SKB, 1999b and Skagius *et al.*, 1999/. These data are compiled to represent fresh concrete with a pH above 12.4 (controlled by the presence of portlandite) and a high ionic strength of the pore water. Leaching of the concrete will decrease the ionic strength of the water and the pH. A decrease in ionic strength will possibly increase the sorption of elements that sorbs via ion exchange. A decrease in pH will not affect the sorption of other elements as long as some portlandite remains in the concrete and not significantly reduce sorption as long as calcium silicate hydrate (CSH) phases remain and pH is above 10 (see below).

In an assessment of the long-term degradation of concrete in SFR /Höglund, 2001/ it is concluded that the expected chemical changes are slow and that alkaline conditions will be maintained in the concrete during the entire period of 10 000 years (see Section 2.1.2). The development of a pH below 12 in the outermost parts of the concrete structures might imply somewhat lower sorption in those parts. However, as long as calcium silicate hydrate (CSH) phases are remaining the difference should not be large for the elements considered, except for inorganic carbon. This is indicated by the K_d-values that were selected as representative for different stages of concrete leaching in the previous safety assessment of SFR-1 (Allard *et al.*, 1991). This is further discussed in subsection 6.2.5.

In Skagius *et al* /1999/ a K_d-value for carbon in the form of carbonate is given, but it is stated that carbonate would rather precipitate than sorb in concrete systems. In the selection of sorption data for the cementitious near field of a repository for low and intermediate level waste in Switzerland, Bradbury and Sarrot /1995/ derived a fictitious K_d for carbonate by assuming isotope exchange between carbon in the solution and carbon in solid phase. A similar approach is used here to estimate a fictitious K_d for inorganic carbon. This is further described in Section 6.2.3.

Bentonite

The sorption data suggested for the bentonite buffer in the Silo are based on data used in the previous assessment of SFR /Wiborgh and Lindgren, 1987/ and on data suggested by Andersson /1999/ for the recent safety assessment of a deep repository for spent fuel, SR 97 /SKB, 1999a/. The data suggested by Andersson /1999/ builds on data proposed by Yu and Neretnieks /1997/ for compacted bentonite with a dry density in the range

1 600 – 2 000 kg/m^3 and on comments to these data given by Ochs /1997/. Data used in TILA-99 for sorption in compacted bentonite /Vieno and Nordman, 1999/ are also considered for comparison. Sorption data for elements that are not included in these references are derived by making chemical analogies.

In the earlier assessments of SFR conservative values were selected. When here selecting K_d-values for sorption in the bentonite buffer in the Silo, the pessimistic values proposed by Andersson /1999/ for reducing conditions and saline groundwater conditions are considered. This is also the case when reference is given to data in TILA-99, i.e. the data considered are the pessimistic values given for reducing conditions and saline water.

Sand/bentonite mixture

The approach adopted in SR 97 and described in Andersson /1999/ is also here used to derive sorption data for the sand/bentonite backfill. A weighted average is made from the K_d-values selected for bentonite and those selected for sand/gravel fill and the weight proportions of bentonite (10 %) and sand (90 %) in the backfill. This simple approach is selected because of the limited amount of experimental data available on sorption in mixtures of sand and bentonite.

Sand/rock fill

In the analysis of the SFL 3-5 repository, K_d for sand/gravel fill was taken from sorption data for granite derived by Carbol and Engkvist /1997/ and used in the recent safety assessment of a deep repository for spent fuel, SR 97 /SKB, 1999a, Andersson, 1999/. The use of these sorption data derived for SR 97 is here also selected for the rock fills in the repository vaults in SFR. The difference compared to the analysis of SFL 3-5 /SKB, 1999b/ is that the pessimistic values suggested in Andersson /1999/ for saline ground-water are selected instead of the reasonable values that were used in the analysis of SFL 3-5.

6.2.3 Evaluation of data

Cementitious materials

The cementitious materials that can be found in the SFR repository are mainly: structural concrete in buildings and waste packaging, concrete grout used as backfill around the waste packages in the Silo, BMA and BTF vaults and cement mortar used as conditioning material for the waste. The same set of sorption data is suggested for all these materials for the whole time period and in all the calculation cases that are analysed within the Base scenario (see Section 2.1.5). This is also the case for the calculation cases defined for other scenarios except for the scenario assuming large quantities of chemicals/complexing agents in the repository. The data suggested for this calculation case are given and motivated in Section 6.3.

The selected K_d-values are given in Table 6-2. These values are the same as those used in the preliminary safety assessment of the SFL 3-5 repository and the background to the values are given in Skagius *et al* /1999/. A few comments to the selected values are given below together with a comparison with K_d-values assumed in the previous safety assessment of SFR. In addition, comparisons are made with K_d-values recommended by Bradbury and Sarrot /1995/, Bradbury and van Loon /1998/ and by Savage *et al* /2000/ for cementitious materials under reducing conditions and pH $\geq$ 12.5.

Carbon (C). In the earlier safety assessment of SFR a K_d of 5 m^3/kg was assumed for sorption of carbon in the form of carbonate in concrete with a pH above 12.5 /Allard *et*

al., 1991/. For a partially leached concrete with a pH above 11 a K_d of 1 m^3/kg was selected /Allard *et al.,* 1991 and Wiborgh and Lindgren, 1987/. The K_d-value selected here and originally proposed by Skagius *et al* /1999/ for Carbon in the form of carbonate is 0.2 m^3/kg, although noting that the retention of carbonate rather is due to precipitation than sorption. Bradbury and Sarrot /1995/ propose that the dominant removal mechanism of radioactive carbonate from the solution is isotope exchange with solid calcium carbonate. They further suggest that an effective sorption coefficient can be calculated as the ratio between the quantity of carbonate contained in the cement and the solubility limit of calcium carbonate in the pore water. For safety assessment it is proposed that the so obtained sorption coefficient is reduced by a factor of 10, which would imply that only 10 % of the mass of solid carbonate is available for isotope exchange. Using the approach suggested by Bradbury and Sarrot /1995/ and data for the cement in structural concrete in SFR would give an effective sorption coefficient of 4.5 m^3/kg at pH 13 (quantity of carbonate in cement = 0.027 mole/kg, concentration of carbonate in solution = 0.006 mol/m^3). Assuming a 10 times reduction due to limited access of the solid carbonate would then give a K_d of 0.45 m^3/kg at pH 13. According to Bradbury and Sarrot /1995/ the K_d will increase with decreasing pH. The K_d of 0.2 m^3/kg as proposed in Skagius *et al* /1999/ is of the same order of magnitude and using this value would then not over-estimate the sorption of inorganic carbon. The selected value is also lower than the best estimate K_d of inorganic carbon given in Savage *et al* /2000/. They propose a K_d of 0.5 m^3/kg for carbon in the form of carbonate in cement/concrete that is not depleted of portlandite.

For other forms of carbon, e.g. organic compounds, a $K_d = 0$ selected.

Chlorine (Cl). Cl has not been considered in earlier safety assessments of SFR and consequently no sorption data are available in Wiborgh and Lindgren /1987/. The value selected here, $K_d = 0.006$ m^3/kg, is the same value that Skagius *et al* /1999/ proposed based on experimental results. Bradbury and Sarrot /1995/ proposed a K_d of 0.02 m^3/kg for Cl. Bradbury and Van Loon /1998/ revised this value and suggested a lower value, $K_d = 0.005$ m^3/kg, in order to take into account a potentially high chloride concentration in the pore water of the cement. Savage *et al* /2000/ give a best estimate K_d for Cl that is 0.001 m^3/kg. The K_d selected here is similar to the value proposed by Bradbury and Van Loon /1998/, but slightly higher than the value proposed by Savage *et al* /2000/.

Iodine (I). In the earlier assessments of SFR a K_d of 0.03 m^3/kg was assumed for sorption of I on cement/concrete at a pH above 12.5 /Allard *et al.,* 1991/. For a partially leached concrete with a pH above 11, a K_d of 0.003 m^3/kg was used /Allard *et al.,* 1991 and Wiborgh and Lindgren, 1987/. Based on experimental results, Skagius *et al.* /1999/ proposed a K_d of 0.003 m^3/kg, which also is the value selected here. Bradbury and Sarrot /1995/ proposed a K_d of 0.002 m^3/kg, which later was revised to 0.01 m^3/kg by Bradbury and Van Loon /1998/. The best estimate value given by Savage *et al.* /2000/ is 0.02 m^3/kg. In comparison with these more recent data, the value suggested here for cement/concrete in SFR is low.

Molybdenum (Mo) and Selenium (Se). These elements were not considered in the previous assessment of SFR. Based on recent experiments, a K_d of 0.006 m^3/kg for sorption of Mo was proposed by Skagius *et al.* /1999/. The same value was also chosen for Se because both elements are expected to be present as anionic species under reducing conditions. This K_d-value is also here selected for sorption of both Mo and Se in cement/concrete in SFR. Bradbury and Van Loon /1998/ propose a $K_d = 0$ for both elements because of the absence of relevant experimental data and because of the anionic form of these species. Savage *et al* /2000/ give a best estimate K_d of 0.01 m^3/kg

for Mo(VI) and $K_d = 0.2$ m^3/kg for Mo(III) based on the use of Cr as a chemical analogue. A best estimate K_d of 0 for sorption of Se is given by Savage *et al*. /2000/. These data indicate that the K_d selected for sorption of Mo probably not are overestimated while a more pessimistic choice of K_d for Se would be to assume zero sorption.

Tritium (H). Skagius *et al* /1999/ propose $K_d = 0$ for sorption of tritium because it probably will be present as tritiated water. Bradbury and Sarrot /1995/ and Bradbury and Van Loon /1998/ propose the same value.

Cesium (Cs) and Silver (Ag). In the previous safety assessments of SFR, K_d-values of 0.001 m^3/kg /Wiborgh and Lindgren, 1987/ as well as of 0.002 m^3/kg (pH above 12.5, high ionic strength) and 0.1 m^3/kg (pH above 11, lower ionic strength) /Allard *et al*., 1991/ have been assumed. Skagius *et al*. /1999/ select a $K_d = 0.001$ m^3/kg, which is the same value that originally was given by Wiborgh and Lindgren /1987/ and which also is the value that here is selected for sorption of Cs on cement/concrete in SFR. Bradbury and Sarrot /1995/ and Bradbury and Van Loon /1998/ recommend a somewhat higher value, $K_d = 0.002$ m^3/kg for high pH and high ionic strength and a further 10 times higher value, $K_d = 0.02$ m^3/kg for a cementitious system where the highly soluble alkali hydroxides are removed. Savage *et al* /2000/ give a best estimate K_d of 0.001 m^3/kg, i.e. the same value as here is proposed for sorption of Cs in cement/concrete in SFR.

Silver has not been considered in the previous safety assessment of SFR. Here a K_d of 0.001 m^3/kg is selected in accordance with the value proposed by Skagius *et al* /1999/. This value was derived by assuming that sorption of Ag would be similar to sorption of Cs. Bradbury and Sarrot /1995/ recommend a K_d of 0.001 m^3/kg for sorption of Ag, i.e. the same value as here is selected for sorption of Ag on cement/concrete in SFR.

Nickel (Ni), Cobalt (Co) Palladium (Pd) and Cadmium (Cd). In the previous safety assessments of SFR a K_d of 0.5 m^3/kg /Wiborgh and Lindgren, 1987/ and of 1 m^3/kg /Allard *et al.,* 1991/ was assumed for sorption of Ni and Co. Pd and Cd were not considered in these assessments. In Skagius *et al* /1999/ a K_d of 0.04 m^3/kg is proposed for sorption of Ni. This value is based on experiments where care was taken to avoid precipitation and sorption on experimental equipment. Due to the expected similar sorption behaviour to Ni, the same K_d was also proposed for sorption of Co, Pd and Cd. Bradbury and Sarrot /1995/ and Bradbury and Van Loon /1998/ recommend a K_d of 0.1 m^3/kg for sorption of both Ni and its chemical analogues Co and Pd. Savage *et al* /2000/ give a best estimate K_d of 0.1 m^3/kg for Ni and 0.5 m^3/kg for Pd. Compared to these data, the K_d-value of 0.04 m^3/kg selected for sorption of Ni, Co, Fe, Pd and Cd on cement/concrete in SFR is low.

Tin (Sn). Tin was not considered in the previous safety assessments of SFR. Skagius *et al* /1999/ propose a $K_d = 0.5$ m^3/kg considering potential problems with solubility and formation of colloids in the experiments from which data are reported. This value is also suggested here for sorption of Sn in cement/concrete in SFR. Savage *et al* /2000/ give the same value as a best estimate for sorption of Sn, while Bradbury and Sarrot /1995/ and Bradbury and Van Loon /1998/ recommend a higher value, $K_d = 1$ m^3/kg.

Strontium (Sr) and Radium (Ra). Sr was considered in the earlier assessments of SFR. Originally a K_d of 0.001 m^3/kg was assumed for fresh and leached, but not chemically degraded, concrete /Wiborgh and Lindgren, 1987/. This value was revised by Allard *et al*. /1991/ to $K_d = 0.002$ m^3/kg for a concrete with pH above 12.5 and high ionic strength and $K_d = 0.02$ m^3/kg for a concrete with pH above 11 and lower ionic strength. For fresh concrete, Skagius *et al*. /1999/ propose the same value as originally

assumed by Wiborgh and Lindgren /1987/, i.e. $K_d = 0.001$ m^3/kg. This value is also selected here for both the early stage with high ionic strength in the concrete and for later stages when the ionic strength has decreased. The same value is recommended by Bradbury and Sarrot /1995/ and Bradbury and Van Loon /1998/, while Savage *et al* /2000/ give a best estimate K_d that is slightly higher, $K_d = 0.005$ m^3/kg.

In accordance with the value proposed by Skagius *et al.* /1999/ a K_d of 0.05 m^3/kg is selected for sorption of Ra in cement/concrete in SFR. The same value is recommended by Bradbury and Sarrot /1995/ and by Bradbury and Van Loon /1998/ and also given by Savage *et al.* /2000/ as the best estimate K_d for sorption of Ra.

Niobium (Nb). In the previous safety assessments of SFR K_d-values of 0.1 m^3/kg /Wiborgh and Lindgren, 1987/ and 2 m^3/kg /Allard *et al.,* 1991/ were assumed. Skagius *et al.* /1999/ selected a K_d of 0.5 m^3/kg, which is a value in the lower range of the large span in experimental data that has been reported in the literature since 1990. This value is selected here for sorption of Nb in cement/concrete in SFR. Bradbury and Sarrot /1995/ recommended the same value, but Bradbury and Van Loon /1998/ revised the value to 1 m^3/kg with reference to experiments at very low Nb concentrations that confirm high sorption of Nb. Savage *et al.* /2000/ gives a best estimate K_d of 0.5 m^3/kg for sorption of Nb.

Americium (Am) and Curium (Cm). The K_d-values assumed in the earlier assessments of SFR for sorption of Am and Cm are 1 m^3/kg /Wiborgh and Lindgren, 1987/ and 5 m^3/kg /Allard *et al.*, 1991/. Skagius *et al* /1999/ selected a K_d of 1 m^3/kg for sorption of Am and Cm with reference to an experiment with Am sorption that was carried out with very low starting concentration, but also noting that other experiments indicate much higher values. The value selected by Skagius *et al.* /1999/ is also selected here for sorption of Am and Cm on cement/concrete in SFR. Bradbury and Sarrot /1995/ recommended a K_d of 5 m^3/kg for sorption of Am and Cm. Bradbury and Van Loon /1998/ revised the value down to 1 m^3/kg referring to the same experiments with low starting concentration of Am as mentioned in Skagius *et al.* /1999/. Savage *et al.* /2000/ give a best estimate K_d of 5 m^3/kg for sorption of Am and Cm.

Samarium (Sm), Europium (Eu) and Holmium (Ho). None of these lanthanides were considered in the previous safety assessments of SFR. Skagius *et al.* /1999/ selected a K_d of 5 m^3/kg for sorption of these lanthanides. This value was chosen based on experiments with sorption of Pm that gave K_d-values larger than 20 m^3/kg, but also taking into account the large uncertainties in determining high K_d:s. This value is also selected here for sorption of Sm, Eu and Ho on cement/concrete in SFR. No recommended K_d-values for these lanthanides are given in Bradbury and Sarrot /1995/ or by Bradbury and Van Loon /1998/. Savage *et al.* /2000/ give a reference to an experiment with sorption of Eu on cement powder over a short contact period that yielded a K_d of 2.4 m^3/kg, but they do not give any best estimate K_d for sorption of lanthanides.

Uranium (U), Neptunium (Np) and Plutonium (PU). Of these actinides, only Pu was considered in the previous assessments of SFR and the K_d assumed was originally 1 m^3/kg /Wiborgh and Lindgren, 1987/. This value was later revised to 5 m^3/kg /Allard *et al.*, 1991/. This latter value is also selected by Skagius *et al.* /1999/ with reference to a number of experiments where the K_d-values obtained usually are larger than 10 m^3/kg. For sorption of U, Np and Pu on cement/concrete in SFR, the same $K_d = 5$ m^3/kg is selected. The same value is also recommended by Bradbury and Sarrot /1995/, by Bradbury and Van Loon /1998/ and by Savage *et al.* /2000/.

Technetium (Tc) and Zirconium (Zr). In the previous assessments of SFR a K_d of 0.1 m^3/kg for sorption of Tc(IV) was originally assumed /Wiborgh and Lindgren, 1987/. Allard *et al.* /1991/ revised this value to 2 m^3/kg. Skagius *et al* /1999/ conclude that the sorption of Tc(IV) and Zr would be high, in analogy with the sorption of the tetravalent actinides. Despite this, they cautiously select a K_d of 0.5 m^3/kg for sorption of both Zr and Tc(IV) based on an experimental value on Zr sorption reported in the literature. This value is also selected here for sorption of Tc(IV) and Zr on cement/concrete in SFR. Bradbury and Sarrot /1995/ and Bradbury and Van Loon /1998/ recommend a K_d of 5 m^3/kg for sorption of Zr and 1 m^3/kg for sorption of Tc(IV). The same values are given by Savage *et al.* /2000/ as best estimate K_d for sorption of Zr and Tc(IV), but they also note that a K_d of 1 m^3/kg for Tc(IV) is low and that a value of 5 m^3/kg is justified based on the analogous behaviour to Th.

Bentonite

The sorption coefficients selected for the bentonite buffer in the Silo are given in Table 6-3. These data are applicable for reducing conditions and saline water and a short motivation to the selected data are given in the following paragraphs. As mentioned earlier in Section 6.2.2, the main source for the selected sorption data is the pessimistic case values given in Andersson /1999/ that builds on K_d-values proposed by Yu and Neretnieks /1997/ and Ochs /1997/. For comparison, data assumed in the earlier safety assessment of SFR and the pessimistic values of the sorption distribution coefficient in compacted bentonite that were assumed in TILA-99 for reducing and saline conditions /Vieno and Nordman, 1999/ are given.

Carbon (C), Chlorine (Cl) and Iodine (I). In the earlier assessments of SFR, $K_d = 0$ was assumed for sorption of carbon, both as carbonate and in organic form, and also for iodine in bentonite /Wiborgh and Lindgren, 1987/. Andersson /1999/ propose $K_d = 0$ for sorption of both inorganic and organic carbon in bentonite as well as for sorption of chlorine and iodine. This value is also selected here for sorption of these elements in the bentonite in the Silo.

Zero sorption of these elements was also assumed in TILA-99 /Vieno and Nordman, 1999/.

Molybdenum (Mo) and Selenium (Se). Molybdenum and Selenium were not considered in the previous assessments of SFR. The realistic value suggested by Andersson /1999/ for sorption of Se is $K_d = 0.003$ m^3/kg and the pessimistic value is $K_d = 0$ m^3/kg. This latter value is selected here for sorption of Se in the bentonite barrier in the Silo. Since Mo, likewise to Se, is expected to be present in anionic form, zero sorption is selected also for Mo.

In TILA-99, zero sorption was assumed for Se as a conservative value under saline conditions and the realistic value reported is 0.005 m^3/kg /Vieno and Nordman, 1999/.

Tritium (H). Neither Wiborgh and Lindgren /1987/ nor Andersson /1999/ suggest any sorption value for tritium. However, in the compilation of experimental data made by Yu and Neretnieks /1997/, a $K_d = 0$ from an experiment with Na-bentonite with a density of 200 kg/m^3 is given /Miyahara *et al.*, 1991/. Since tritium probably will exists as tritiated water no sorption is expected and a $K_d = 0$ is selected.

Cesium (Cs) and Silver (Ag). In the earlier assessment of SFR a K_d of 0.2 m^3/kg was used for Cs sorption in unaltered bentonite and a K_d of 0.005 m^3/kg for sorption of Cs in bentonite that is chemically affected by components from the concrete /Wiborgh and Lindgren, 1987/. The data given in Andersson /1999/ for sorption of Cs under saline

conditions are a realistic K_d of 0.05 m^3/kg and a pessimistic K_d-value of 0.005 m^3/kg. For sorption of Ag, Andersson /1999/ propose $K_d = 0$. It is possible that Ag will be present predominantly in the +1 state in the bentonite and likewise to Cs sorb via an ion-exchange mechanism. In that case, the same K_d as for Cs could be expected. However, in accordance with the pessimistic values proposed in Andersson /1999/ a K_d of 0.005 m^3/kg is selected for sorption of Cs and $K_d = 0$ for sorption of Ag in the bentonite in the Silo.

In TILA-99, a conservative K_d of 0.02 m^3/kg was assumed for sorption of Cs under saline conditions, i.e. a 4 times higher value than here suggested for sorption of Cs in the bentonite in the Silo. The realistic value reported for saline conditions is 0.2 m^3/kg /Vieno and Nordman, 1999/.

Nickel (Ni), Cobalt (Co) and Cadmium (Cd). In the earlier assessment of SFR the same K_d of 0.2 m^3/kg was used for sorption of Ni and Co in unaltered bentonite due to their expected similar behaviour /Wiborgh and Lindgren, 1987/. For sorption in bentonite affected by components from the concrete a 10 times lower value was assumed, $K_d = 0.02$ m^3/kg /Wiborgh and Lindgren, 1987/. Andersson /1999/ propose a realistic K_d of 0.1 m^3/kg and a K_d-value of 0.02 m^3/kg for sorption of Ni in the pessimistic case, which also is the value selected here for sorption of Ni in bentonite in the Silo. The same value is selected also for Co.

In TILA-99, the conservative value assumed for sorption of Ni under saline conditions is $K_d = 0.001$ m^3/kg, i.e. 20 times lower than the value selected here for sorption of Ni in the bentonite in the Silo. The realistic value reported is 0.01 m^3/kg /Vieno and Nordman, 1999/.

No data are available in Wiborgh and Lindgren /1987/ or in Andersson /1999/ on the sorption of Cd. However, Cd is expected to behave similar to Ni both what concerns sorption on concrete /Skagius *et al.*, 1999/ and on granite /Carbol and Engkvist, 1997/. Therefore, the same K_d-value as for Ni is here suggested for Cd sorption on bentonite.

Palladium (Pd). Palladium was not considered in the earlier assessments of SFR. Andersson /1999/ propose a K_d-value of 0 m^3/kg for Pd sorption in compacted bentonite in the pessimistic case in accordance with the pessimistic value proposed by Yu and Neretnieks /1997/ for saline conditions. The realistic value for saline conditions proposed by Yu and Neretnieks /1997/ is 0.01 m^3/kg. According to Skagius *et al* /1999/ and Carbol and Engkvist /1997/, sorption of Pd in concrete and in granite is expected to be similar to the sorption of Ni. If this also is the case for sorption in bentonite, the value given in Andersson /1999/ is very pessimistic. This is also a remark given by Ochs /1997/ to the values proposed by Yu and Neretnieks /1997/ for sorption of Pd. Despite this, zero sorption of Pd in the bentonite in the Silo is also here selected, but with the remark that this probably is a very pessimistic choice.

In TILA-99, a conservative K_d of 0.001 m^3/kg is assumed for sorption of Pd under saline conditions /Vieno and Nordman, 1999/, i.e. the same value as is assumed for sorption of Ni under saline conditions. The realistic value reported is 0.1 m^3/kg /Vieno and Nordman, 1999/.

Tin (Sn). No sorption data for Sn are given in Wiborgh and Lindgren /1987/ since Sn was not considered in the previous assessments of SFR. Thus, the pessimistic value given in Andersson /1999/, $K_d = 0.01$ m^3/kg, is here selected for sorption of Sn in the bentonite in the Silo in SFR. For comparison, the realistic value proposed by Yu and Neretnieks /1997/ is $K_d = 3$ m^3/kg.

The conservative value assumed in TILA-99 is $K_d = 0.001$ m^3/kg for sorption of Sn in compacted bentonite under saline conditions (Vieno and Nordman, 1999). The realistic value reported is 0.2 m^3/kg (Vieno and Nordman, 1999).

Strontium (Sr) and Radium (Ra. In the earlier assessment of SFR a K_d of 0.1 m^3/kg was assumed for sorption of Sr in unaltered bentonite and a K_d of 0.001 m^3/kg for sorption in bentonite that is affected by the concrete /Wiborgh and Lindgren, 1987/. This latter value, $K_d = 0.001$ m^3/kg, is also proposed by Andersson /1999/ as a pessimistic case value for sorption of both Sr and Ra. Therefore, this value is selected here for Sr and Ra sorption in bentonite in SFR. For comparison, Yu and Neretnieks /1997/ propose $K_d = 0.01$ m^3/kg as a realistic value for sorption of Sr in bentonite under saline conditions.

In TILA-99, the conservative K_d-values assumed for saline conditions are 0.001 m^3/kg for sorption of Sr and 0.002 m^3/kg for sorption of Ra /Vieno and Nordman, 1999/, i.e. values very similar to those proposed here for the bentonite in the Silo. The realistic values reported are 0.004 m^3/kg for Sr and 0.01 m^3/kg for Ra /Vieno and Nordman, 1999/.

Niobium (Nb). In the earlier assessment of SFR, a K_d of 0.1 m^3/kg was used for sorption of Nb in unaltered bentonite and $K_d = 0.05$ m^3/kg for sorption of Nb in bentonite that is affected by the concrete /Wiborgh and Lindgren, 1987/. Andersson /1999/ propose zero sorption of Nb for the pessimistic case and a realistic K_d of 0.2 m^3/kg for sorption of Nb in bentonite. In accordance with the strategy for selecting data, the pessimistic assumption of zero sorption of Nb in the bentonite in the Silo is here adopted.

The conservative K_d assumed in TILA-99 for sorption of Nb is 0.02 m^3/kg and the realistic value given is 1 m^3/kg /Vieno and Nordman, 1999/.

Americium (Am) and Curium (Cm). In the earlier safety assessments of SFR a K_d of 1 m^3/kg was assumed for sorption of Am and Cm in unaltered bentonite and a K_d of 0.5 m^3/kg in bentonite that is affected by the concrete /Wiborgh and Lindgren, 1987/. Andersson /1999/ propose a realistic K_d-value of 3 m^3/kg and a pessimistic value of 1 m^3/kg for Am and Cm sorption. This latter value is here selected for sorption of Am and Cm in the bentonite in the Silo.

In TILA-99, the conservative K_d-value assumed for Am and Cm is 0.3 m^3/kg and the realistic value given is 3 m^3/kg for both Am and Cm /Vieno and Nordman, 1999/.

Samarium (Sm), Europium (Eu) and Holmium (Ho). No sorption data are given for these lanthanides in Wiborgh and Lindgren /1987/ since they were not considered in the previous assessments of SFR. The realistic and pessimistic K_d-values proposed by Andersson /1999/ for Sm and Ho are 1 m^3/kg and 0.2 m^3/kg, respectively. Because of the large similarity in chemical behaviour of the lanthanides the pessimistic value given in Andersson /1999/, i.e. $K_d = 0.2$ m^3/kg, is here selected for the sorption of all lanthanides in the bentonite in the Silo.

The conservative K_d-value assumed for Sm in TILA-99 is 0.2 m^3/kg and the realistic value given is 1 m^3/kg /Vieno and Nordman, 1999/.

Plutonium (Pu). In the earlier assessments of SFR, a $K_d = 1$ m^3/kg was assumed for sorption of Pu in unaltered bentonite and 0.5 m^3/kg in bentonite affected by concrete /Wiborgh and Lindgren, 1987/. Andersson /1999/ propose a realistic K_d of 3 m^3/kg and

a pessimistic value of 1 m^3/kg for sorption of Pu under reducing conditions. This latter value is also selected here for sorption of Pu in the bentonite in the Silo.

In TILA-99, a conservative K_d of 0.3 m^3/kg is assumed and the realistic value given is 3 m^3/kg /Vieno and Nordman, 1999/.

Neptunium (Np). Neptunium was not considered in the previous assessments of SFR. Andersson /1999/ propose a realistic K_d of 3 m^3/kg and a pessimistic value of 0.1 m^3/kg for sorption of Np. This pessimistic value is also here selected for sorption of Np in the bentonite in the Silo.

The conservative K_d-values assumed in TILA-99 is 0.1 m^3/kg for Np and the realistic value given is 10 times higher /Vieno and Nordman, 1999/.

Uranium (U). Uranium was not considered in the previous assessments of SFR. The realistic and pessimistic values proposed in Andersson /1999/ for sorption of U are 1 m^3/kg and 0.01 m^3/kg, respectively. Here the pessimistic value according to Andersson /1999/ is selected for sorption of U in the bentonite in the Silo.

In TILA-99, a conservative K_d of 0.05 m^3/kg is assumed for sorption of U and the realistic value given is 10 times higher, i.e. 0.5 m^3/kg /Vieno and Nordman, 1999/.

Zirconium (Zr). Zirconium was not considered in the previous assessments of SFR. Andersson /1999/ propose a realistic K_d of 2 m^3/kg and a pessimistic value of 0.05 m^3/kg for sorption of Zr. This latter value is also here selected for sorption of Zr in the bentonite in the Silo in SFR.

In TILA-99, a conservative K_d of 0.2 m^3/kg is assumed for sorption of Zr and the realistic value given is 1 m^3/kg /Vieno and Nordman, 1999/.

Technetium (Tc). The K_d assumed in the previous assessment of SFR for sorption of Tc(IV) is 0.05 m^3/kg in unaltered bentonite and 0.005 m^3/kg in bentonite that is chemically altered by components from the concrete /Wiborgh and Lindgren, 1987/. The realistic K_d-value proposed by Andersson /1999/ for sorption of Tc(IV) is 0.1 m^3/kg and the pessimistic value is 0.01 m^3/kg. This latter value is also here selected for sorption of Tc(IV) in bentonite in the Silo.

The conservative K_d-value assumed in TILA-99 for sorption of Tc(IV) is 0.01 m^3/kg and the realistic value given is 10 times higher, i.e. 0.1 m^3/kg /Vieno and Nordman, 1999/.

Sand/bentonite mixture

A mixture of sand and bentonite with the proportions 10 % bentonite and 90 % sand by weight will be used as backfill in the bottom and in the top of the Silo. To derive sorption data for the sand/bentonite backfill, a weight-based average is made from the K_d-values suggested for bentonite in Table 6-3and those suggested for gravel fill in Table 6-5. The so derived K_d-values are given in Table 6-4.

Rock fill

The rock fill that will be used in SFR is here assumed to be similar to the sand/gravel fill defined for the SFL 3-5 repository concept. In the analysis of SFL 3-5 sorption data for sand/gravel fill in the different repository parts were assumed to be those compiled by Carbol and Engkvist /1997/ for granite for the SR 97 safety assessment /SKB, 1999a/. The same approach are used here, with the difference that the values for saline groundwater suggested for the pessimistic case calculations in SR 97 /Andersson, 1999/

are selected instead of the reasonable values that were adopted in the SFL 3-5 analysis /SKB, 1999b and Skagius *et al.*, 1999/. For elements that were not considered in SR 97, data are selected based on the same chemical analogies that were used to select data for the SFL 3-5 analysis. The data selected for sorption in sand/gravel fill in the repository vaults in SFR are compiled in Table 6-5.

6.2.4 Selected data

In this subsection the selected K_d-values for sorption on the different engineered barriers in SFR are tabulated. The background to the selected data is given in the previous subsection.

Table 6-2. Selected K_d-values for sorption on cement/concrete in SFR.

Ox. state[1]	Element	K_d (m^3/kg)
M(I)	H	0
	Cs, Ag	0.001
M(II)	Ni, Co, Pd, Cd	0.04
	Sr	0.001
	Ra	0.05
M(II/IV)	Sn	0.5
M(III)	Am, Cm	1
	Sm, Eu, Ho	5
M(IV)	U, Np, Pu	5
	Zr, Tc	0.5
	C(inorg.)	0.2
	C(org.)	0
M(V)	Nb	0.5
M(VI)	Mo	0.006
M(-I)	Cl	0.006
	I	0.003
M(-II,IV,VI)	Se	0.006

[1] *oxidation state for major ionic species at reducing Eh and pH 7-14*

Table 6-3. Selected K_d-values for sorption in bentonite in SFR

Ox. state	Element	K_d (m³/kg)	Reference/Comment
M(I)	H	0	As water molecules
	Cs	0.005	Pessimistic value, saline water, Andersson /1999/
	Ag	0	Pessimistic value, saline water, Andersson /1999/
M(II)	Ni	0.02	Pessimistic value, saline water, Andersson /1999/
	Co, Cd	0.02	In analogy with Ni
	Pd	0	Pessimistic value, saline water, Andersson /1999/
	Sr, Ra	0.001	Pessimistic value, saline water, Andersson /1999/
M(II/IV)	Sn	0.01	Pessimistic value, saline water, Andersson /1999/
M(III)	Am, Cm	1	Pessimistic value, saline water, Andersson /1999/
	Sm, Ho	0.2	Pessimistic value, saline water, Andersson /1999/
	Eu,	0.2	In analogy with Sm and Ho
M(III,IV)	Pu	1	Pessimistic value, saline water, Andersson /1999/
M(IV)	Np	0.1	Pessimistic value, saline water, Andersson /1999/
	U	0.01	Pessimistic value, saline water, Andersson /1999/
	Zr	0.05	Pessimistic value, saline water, Andersson /1999/
	Tc	0.01	Pessimistic value, saline water, Andersson /1999/
	C(inorg. and org.)	0	Andersson /1999/
M(V)	Nb	0	Pessimistic value, saline water, Andersson /1999/
M(VI)	Mo	0	In analogy with Se
M(-I)	Cl, I	0	Andersson /1999/
M(-II,IV,VI)	Se	0	Pessimistic value, saline water, Andersson /1999/

Table 6-4. Selected K_d-values for sorption on 90/10 sand/bentonite in SFR. Calculated from Tables 6-3 and 6-5.

Ox. state	Element	K_d (m³/kg)
M(I)	H	0
	Cs	0.01
	Ag	0.009
M(II)	Ni, Co, Cd	0.01
	Pd	0.0009
	Sr	0.0002
	Ra	0.009
M(II/IV)	Sn	0.001
M(III)	Am, Cm	1
	Sm, Ho, Eu	0.9
M(III,IV)	Pu	1
M(IV)	Np, U	0.9
	Zr	0.5
	Tc	0.3
	C (inorg.)	0.0005
	C (org.)	0
M(V)	Nb	0.5
M(VI)	Mo	0
M(-I)	Cl, I	0
M(-II,IV,VI)	Se	0.0005

Table 6-5. Selected K_d-values for sorption on rock fill (sand/gravel) in SFR

Ox. state	Element	K_d (m³/kg)	Reference/Comment
M(I)	H	0	Skagius et al. /1999/
	Cs, Ag	0.01	Pessimistic value, saline water, Andersson /1999/
M(II)	Ni, Co, Cd	0.01	Pessimistic value, saline water, Andersson /1999/
	Pd	0.001	Pessimistic value, saline water, Andersson /1999/
	Sr	0.0001	Pessimistic value, saline water, Andersson /1999/
	Ra	0.01	Pessimistic value, saline water, Andersson /1999/
M(II/IV)	Sn	0	Andersson /1999/
M(III)	Am, Cm, Sm, Ho, Eu	1	Pessimistic value, saline water, Andersson /1999/
M(III,IV)	Pu	1	Pessimistic value, saline water, Andersson /1999/
M(IV)	Np, U	1	Pessimistic value, saline water, Andersson /1999/
	Zr	0.5	Pessimistic value, saline water, Andersson /1999/
	Tc	0.3	Pessimistic value, saline water, Andersson /1999/
	C(inorg.)	0.0005	Pessimistic value, saline water, Andersson /1999/
	C(org.)	0	Skagius et al., 1999
M(V)	Nb	0.5	Pessimistic value, saline water, Andersson /1999/
M(VI)	Mo	0	Skagius et al., 1999
M(-I)	Cl, I	0	Andersson /1999/
M(-II,IV,VI)	Se	0.0005	Pessimistic value, saline water, Andersson, 1999

6.2.5 Data uncertainties

Cement/concrete

Sorption on cement/concrete is dependent on the stage of leaching of the cement/concrete. The values selected for sorption on cement/concrete in SFR are primarily applicable for the stage of leaching when portlandite is still remaining, i.e. pH is still above 12. However, it is judged that the values are selected cautiously enough to be representative also for lower pH. This is supported by a comparison of the selected data with the data selected by Allard *et al.* /1991/ and used in previous assessments of SFR. The data selected are lower than the earlier data for all elements reported, except for inorganic carbon, even for a pH as low as 10.4. Bradbury and Sarrot /1995/ reports proposed K_d-values also for a pH below 12.5 that represents a stage where the cement is depleted of portlandite and CSH-phases are leached. For some of the elements these sorption values are lower than those selected for SFR, but for other elements the values are higher. According to Savage *et al.* /2000/, these values proposed by Bradbury and Sarrot /1995/ should rather be representative for sorption in a natural rock-water systems (pH 8-9) in which a low sorbing mineral such as quartz dominate. This together with the relatively small amount of concrete that is expected to be exposed to extensive leaching implies that the values selected for sorption on cement/concrete should be applicable for the whole time period considered in the analysis without overestimating the effect of sorption.

Bentonite and sand/bentonite

The dry density of the bentonite barrier around the Silo in SFR is 1 050 kg/m³ /Wiborgh and Lindgren, 1987/, i.e. lower than the density for which the selected sorption data are derived. There are experimental data available that indicate that the density of the bentonite may affect sorption. Yu and Neretnieks /1997/ refer to experiments in compacted Na-bentonite carried out by Oscarson *et al* /1994/ that show a decrease in sorption of Cs with increasing density in the density range 500 to 1500 kg/m³. However,

they also refer to experiments where no difference in sorption coefficients for Sr and Cs were found between batch experiments with suspended bentonite particles and experiments with bentonite compacted to a high density /Eriksen and Janson, 1996/. In a literature review made by Muurinen *et al* /1994/ similar results are reported. Experiments carried out by Sato *et al* /1992/ showed a decrease in the sorption coefficient for Sr, Tc, I and Cs with increasing density of Na bentonite in the density range 200 to 2000 kg/m^3 while the sorption of Np and Am remained rather constant. Despite the unclear dependence of sorption on bentonite density these results at least indicate that selecting sorption data derived for bentonite with a higher density should not overestimate the effect of sorption.

The composition of the pore water in the bentonite as well as the mineralogy is affecting the sorption of species in the bentonite. The sorption data that are suggested in Andersson /1999/ are representative for sodium bentonite and a pH in the range 8 to 10. In the Silo in SFR, the bentonite will interact with both dissolved components in the groundwater and components leached from the concrete structure. This is discussed in Section 2.1.2 where it is concluded that it is reasonable to assume that the pH in the pore water of both the bentonite and the sand/bentonite barriers in the Silo may well be above 10. Since sorption of many elements is pH dependent, uncertainties are introduced by here assuming sorption data for a pH in the interval 8 to 10. However, Andersson /1999/ notes that the impact of pH above the range for which data are given probably is much less than the impact of a pH below that range.

Another impact of dissolved components in the groundwater and components leached from the concrete is the change in mineralogy of the bentonite (see Section 2.1.2). Ion exchange will gradually convert the sodium bentonite to calcium, potassium and magnesium bentonite. Reaction with alkaline concrete water may form reaction products like CSH-minerals and zeolites (see e.g. Savage et al. /2001/). The formation of such minerals is not expected to drastically reduce the sorption capacity of the bentonite barrier, since these minerals in themselves may act as good sorbents.

The simple approach used to derive sorption data for sand/bentonite from data on bentonite and on sand/gravel introduce uncertainties in the data. However, since both bentonite data and sand/gravel data are selected in order not to overestimate sorption, the resulting data for sand/bentonite should also be pessimistic in the sense that they do not overestimate sorption.

Rock fill

The data selected are representative for saline groundwater and a pH between 7 and 9 /Carbol and Engkvist, 1997/. These values are judged to be low enough to cover any effects of a potential future increase in pH because of the leaching of the concrete barriers and any reduction in ionic strength of the water that might occur in the future when the groundwater becomes fresh. The reason for this is that an increase in pH and the potential alteration of the rock fill that this can cause rather should increase the sorption capacity of the rock than the opposite. A future decrease in salinity of the water would also imply a higher sorption of those elements that are sensitive to ionic strength.

6.3   Influence of complexing agents on sorption

6.3.1   Complexing agents in SFR

The presence of complexing agents in the repository may decrease the sorption of certain elements in the engineered barriers. The major complexing agents expected in SFR are degradation product of cellulose, isosaccharinic acid (ISA), and

decontamination chemicals like EDTA. A study aimed at estimating the concentration of complexing agents in the different waste types allocated to SFR /Fanger *et al.*, 2001/ has showed that it cannot be excluded that the concentration of complexing agents in a few waste types reaches levels where sorption might be affected.

In regard to ISA, effects on sorption is not expected at concentrations below 10^{-4} M (see e.g. Skagius *et al.* /1999/ and Fanger *et al.* /2001/). With the rather conservative assumptions used in the calculations, this limit is just reached inside the waste packages in two waste types allocated to BMA if ISA sorption in the cement waste matrix is accounted for. If also ISA sorption in the cement in the surrounding waste package is included, the concentration of ISA will be lower than 10^{-4} M. The highest concentration of ISA is obtained in waste packages with bitumenised waste, but bitumen is anyhow not considered as a sorption barrier.

Of the chemicals that can act as complexes for radionuclides, it is only EDTA and sodium capryliminodipropionat (NKP) that possibly, in a few waste types, can reach levels where sorption of divalent ions are affected /Fanger *et al.*, 2001/.

6.3.2 Impact on sorption on cement/concrete

The impact on sorption of ISA is discussed in e.g. Skagius *et al.* /1999/, Fanger *et al.* /2001/ and Savage *et al.* /2001/ where references to a number of experimental and theoretical studies can be found, e.g. Van Loon and Glaus /1998/. These references indicate that the sorption of three and tetravalent elements in cement/concrete is reduced in the presence of ISA at concentrations of the order of 10^{-4} to 10^{-3} M, while an ISA concentration above 10^{-2} M is required before divalent ions are affected. Sorption reduction factors reported by Bradbury and Van Loon /1998/ indicate that sorption of tetravalent actinides could be reduced by a factor of up to 100 if ISA-concentration are above 10^{-3} M, while the sorption of trivalent actinides would probably remain unaffected.

Impact on sorption of the presence of complexing agents such as EDTA, NTA, citric and oxalic acid are reported by Bradbury and Sarrot /1995/. From their results it can be concluded that the sorption of Ni and chemical analogous divalent elements may be reduced in the presence of EDTA at concentrations above 10^{-4} M and in the presence of NTA at concentration above 10^{-2}. At those levels the suggested reduction in sorption is a factor 2 in the presence of EDTA and a factor of 5 in the presence of NTA.

6.3.3 Selected data

Base Scenario calculation cases

The estimated concentrations of EDTA and NTA in the waste packages in SFR indicate that a slight effect on sorption on cement/concrete of divalent Ni and chemical analogous elements in the waste packages cannot be excluded. However, considering that the selected K_d-value for Ni in the absence of complexing agents is 2.5 times lower than the value proposed by Bradbury and Van Loon /1995/ and 25 times lower than the best estimate suggested by Savage *et al.* /2000/ it is decided to neglect any effect of EDTA and NTA in the Base scenario calculations. The same decision is made for the potential effect on sorption of tetra- and pentavalent elements inside the waste packages of a few waste types for which the ISA concentration may reach levels above 10^{-4} M. Even if the selected K_d-values for most of these elements are the same as those proposed in the references used for comparison (e.g. Savage *et al.* /2000/), these values are still low in comparison with experimental data reported in the literature (see Section 6.2.3).

Other scenarios – chemicals/complexing agents

As a part of the analyses of Other Scenarios, calculation cases are defined to explore the impact of reduced sorption because of the presence of complexing agents. For this purpose it is decided to reduce the K_d-values selected for the Base Scenario calculations with a factor of 100 for tetra- and pentavalent elements and with a factor of 10 for di- and trivalent elements. These factors are selected for sorption reduction in all engineered barriers, i.e. in cement/concrete, bentonite and sand/bentonite and in sand/gravel fill. The resulting K_d-values for the calculation cases with complexing agents are given in Table 6-6.

Comparing these selected reduction factors with the reduction factors proposed for sorption on concrete in the presence of ISA would suggest a concentration of ISA of the order of 10^{-3} to 10^{-2} M. By the use of the sorption isotherm for ISA on cement and the yield of ISA from alkaline degradation of cellulose that is given in Fanger *et al.* /2001/ and the total quantity of cement and water present in a repository vault the quantity of cellulose that would give this concentration of ISA can be back calculated. Such a calculation for BMA reveals that a quantity of about 3200 tonnes of cellulose would be required to reach a concentration of 10^{-3} M and about 4990 tonnes to reach a concentration of ISA of 10^{-2} M. These quantities are about 350 to 550 times more than the actual prognosis of the quantity of cellulose in BMA.

A similar calculation exercise can be made for the assumed reduction factor for Ni and chemically analogous divalent elements. A reduction factor of 10 for these elements would according to Bradbury and Sarrot /1995/ correspond to a concentration of EDTA of about 10^{-2} M. Assuming that this is the average concentration of EDTA in the water in the concrete interior of BMA the total quantity of EDTA in BMA has to be about 12 500 kg. This can be compared with the present estimate of about 3 kg. If it is assumed that sodium capryliminodipropionat (NKP) has similar impact on sorption as EDTA, the quantity of 12 500 kg of EDTA and NKP should be compared with the present estimate of about 197 kg EDTA and NKP /Fanger *et al.*, 2001/.

Table 6-6. Selected K$_d$-values [m^3/kg] for the calculation cases with impact of complexing agents

Ox. state	Element	Concrete	Bentonite	Sand/bentonite	Sand/gravel fill
M(I)[a]	H	0	0	0	0
	Cs	0.001	0.005	0.01	0.01
	Ag	0.001	0	0.009	0.01
M(II)	Ni, Co, Cd	0.004	0.002	0.001	0.001
	Pd	0.004	0	0.00009	0.0001
	Sr[a]	0.001	0.001	0.0002	0.0001
	Ra[a]	0.05	0.001	0.009	0.01
M(II/IV)	Sn	0.005	0.0001	0.00001	0
M(III)	Am, Cm	0.1	0.1	0.1	0.1
	Sm, Ho, Eu	0.5	0.02	0.09	0.1
M(III,IV)	Pu	0.05	0.01	0.01	0.01
M(IV)	Np	0.05	0.001	0.009	0.01
	U	0.05	0.0001	0.009	0.01
	Zr	0.005	0.0005	0.005	0.005
	Tc	0.005	0.0001	0.003	0.003
	C(inorg.)[a]	0.2	0	0.0005	0.0005
	C(org.)[a]	0	0	0	0
M(V)	Nb	0.005	0	0.005	0.005
M(VI)	Mo	0.006	0	0	0
M(-I)	I[a], Cl[a]	0.003	0	0	0
M(-II,IV,VI)	Se[a]	0.006	0	0.0005	0.0005

[a] not affected by complexing agents

6.4   Porosity, diffusivity and density

6.4.1   Data needed

To calculate the radionuclide migration by diffusion through the near-field barriers the near-field model requires values of the effective diffusivity, D_e, and the porosity, ε. These entities are correlated in that the effective diffusivity is dependent on the porosity according to:

$$D_e = D_w \cdot \varepsilon \cdot \frac{\delta}{\tau^2} \tag{6-1}$$

where D_w is the diffusivity of a species in unconfined water [m^2/s], δ is the constrictivity factor that accounts for the narrowing of passages in the pore structure and τ^2 is the tortuosity factor that accounts for the impact on the diffusion length of the winding of the pores.

The transient phase of the diffusion transport is described by the apparent diffusivity, D_a. This entity is calculated in the near-field model from given values of the effective diffusivity, D_e, the porosity, ε, the sorption distribution coefficient, K_d and the bulk density, ρ, of the material according to:

$$D_a = \frac{D_e}{\varepsilon + K_d \rho} \tag{6-2}$$

6.4.2 Data sources and evaluation of data

Cement/concrete

In the previous assessments of SFR, a porosity of 15% and an effective diffusivity of $3\cdot10^{-12}$ m^2/s for fresh *structural concrete* and $3\cdot10^{-11}$ m^2/s for aged structural concrete was used in the calculations of radionuclide release /Wiborgh and Lindgren, 1987/. The same porosity value of 15% was selected for structural concrete in the preliminary assessment of the SFL 3-5 repository concept, but just one value of the effective diffusivity, $1\cdot10^{-11}$ m^2/s, was selected /Skagius *et al.*, 1999/.

The most recent modelling of the possible chemical alteration of structural concrete in SFR indicates porosity changes from about 10% in unaltered, fully hydrated concrete to values in the range 6 – 19% in altered concrete after 10 000 years /Höglund, 2001/. Porosity values above 15% are only achieved within the first 0.1 to 0.2 m from the outer surface of the concrete structures, which is the most degraded part of the concrete. These results do not oppose the assumption of a porosity of 15% made in previous analyses and therefore this value is suggested for the porosity of structural concrete in SFR over the whole time period of 10 000 years.

The effective diffusivity of $1\cdot10^{-11}$ m^2/s in *structural concrete* that was assumed in the preliminary assessment of SFL 3-5 was cautiously selected based on experimental data for unaltered concrete /Skagius *et al.*, 1999/. This value is also selected for the structural concrete in the SAFE analyses. Since the effective diffusivity is dependent on both porosity and the structures of the pores, alteration of the concrete will affect the effective diffusivity. The expected small changes in porosity due to alteration of the concrete will not significantly affect the effective diffusivity in the altered parts. Larger impact on the diffusivity from alteration is expected from changes in pore structure, but the effect is difficult to quantify without access to experimental data. Theoretically, the effective diffusivity could be of the order of 10 times higher in parts where the concrete is totally depleted of all calcium silicate hydrate (CSH) phases compared to the diffusivity in unaltered concrete /Höglund, 2001/. However, only a few cm of the outermost parts of the concrete structures that are not surrounded by bentonite barriers will be totally depleted of CSH during the first 1000 years and at most about 0.2 m during 10 000 years. Because of this, the potential effect of alteration is neglected and an effective diffusivity of $1\cdot10^{-11}$ m^2/s in *structural concrete* is assumed for the whole time period of 10 000 years.

The density of *structural concrete*, as calculated from the mixing proportions of the concrete given in Table 4-8, is 2343.5 kg/m^3. For the calculations of radionuclide release a bulk density of 2300 kg/m^3 for structural concrete in SFR is selected.

Concrete grout is used as backfill around the waste packages in the Silo and around the steel drums in 1BTF. The Silo grout (also used in BMA when appropriate) has a higher w/c ratio and permeability than structural concrete. In earlier assessments of SFR as well as in the preliminary assessment of SFL 3-5 a porosity of 30% was assumed for the type of grout used in the Silo. The porosity calculated by Höglund /2001/ using a hydration model is 30.9%. Using the same hydration model to calculate the porosity of the BTF grout give values of 18.8% for the bottom grout and 20.8% for the top grout (see Table 4-8). For the calculations of radionuclide release a value of 30% is selected for the Silo concrete grout and 20% for the BTF grout, bottom and top.

No experimental diffusivity data are available for the Silo and BTF concrete grouts. In earlier SFR assessments an effective diffusivity of $3\cdot10^{-10}$ m^2/s in the Silo grout was assumed, i.e. a ten times higher value than in aged structural concrete /Wiborgh and

Lindgren, 1987/. The reason to the selection of a higher diffusivity is the higher w/c ratio and thus higher capillary porosity in the Silo grout. The same relation between the effective diffusivity in Silo grout and in structural concrete is assumed for the calculations of radionuclide release in the SAFE project, i.e. an effective diffusivity of $1 \cdot 10^{-10}$ m^2/s is selected for the Silo grout. This value is also selected for the effective diffusivity in the BTF grout even if the w/c ratio (see Table 4-8) points at a value in between the values for structural concrete and Silo grout.

Neither the Silo grout nor the BTF grout is expected to be exposed to any significant alteration during a time period of 10 000 years and the selected values are therefore assumed for the whole time period.

The density of Silo grout, as calculated from the mixing proportions of the concrete given in Table 4-8, is 1993 kg/m^3. For the BTF grout a corresponding calculation gives a density of 2222 kg/m^3 for the bottom part and 2296 – 2354 kg/m^3 for the top part without and with the maximum allowable moisture content in the ballast material, respectively. For the calculations of radionuclide release a bulk density of 2000 kg/m^3 for the Silo grout and 2300 kg/m^3 for the BTF grout (bottom and top) is selected.

Bentonite and sand/bentonite

The bentonite used in the Silo is a sodium bentonite. The slot between the concrete walls and the rock contains pure bentonite while a mixture of 90% sand and 10% bentonite is used for the bottom bed under the concrete structure as well as for a top barrier placed above the concrete lid.

According to earlier safety assessments of SFR, the pure bentonite barrier has a porosity of 61% and the sand/bentonite barriers a porosity of 25% /Wiborgh and Lindgren, 1987/. Based on the results from the modelling carried out by Höglund /2001/ no increase in the porosity of the bentonite barriers are expected as a result of long-term interactions with groundwater and cementitious water. However, a reduction in porosity cannot be excluded. A reduction in porosity would decrease the transport capacity of the barriers and disregarding this would then not underestimate the release of radionuclides. Therefore a porosity of 61% and 25% is selected for pure bentonite and sand/bentonite barriers, respectively, for the whole time period of 10 000 years (see Table 6-10).

The bulk density (dry) of the pure bentonite barrier outside the concrete walls of the Silo varies from 1120 kg/m^3 at the bottom to 950 kg/m^3 at the top /Pusch, 1985/. In the previous safety assessments a bulk density of 1050 kg/m^3 was selected for the entire barrier /Wiborgh and Lindgren, 1987/. The bulk density (dry) of both the bottom and top barrier of a 90/10 mixture of sand and bentonite is 2000 kg/m^3 /Wiborgh and Lindgren, 1987/. The same values of the bulk density as in the previous assessments are here selected for the pure bentonite and the sand/bentonite barriers (see Table 6-10).

In the earlier safety assessments of SFR, an effective diffusivity of $1 \cdot 10^{-10}$ m^2/s was assumed in both the pure bentonite barrier and in the sand/bentonite barriers /Wiborgh and Lindgren, 1987/. In order to confirm these values or find support for the selection of other values, experimentally determined effective diffusivities reported in the literature were reviewed.

The main source for the pure bentonite data is a review of recent experimental data on sorption and diffusion in the literature made by Yu and Neretnieks /1997/. Experimentally determined values of the effective diffusivity, D_e, in bentonite with a bulk density (dry) in the range 800 to 1300 kg/m^3 are compiled in Table 6-7. Results from experiments with deionised and distilled water are not included. Most of the D_e-

values in the table are lower than 10^{-10} m^2/s. The only exceptions are one value for diffusion of Cl in Na-bentonite with a density of 1200 kg/m^3 carried out in 1 M NaCl solution and one value for diffusion of H and one for diffusion of Sr in Ca-bentonite with a density of 1300 kg/m^3 in 0.05 M CaCl$_2$ solution. All these three exceptions are only slightly higher than 10^{-10} m^2/s and therefore it seems to be no reason for changing the value of 10^{-10} m^2/s assumed for diffusion in pure bentonite in the previous assessments based on the D_e-values in Table 6-7.

Table 6-7. Experimentally determined effective (D_e) and apparent (D_a) diffusivity in bentonite with a bulk density (dry) in the range 800 to 1300 kg/m^3.

Element	D_e (m^2/s)	D_a (m^2/s)	Bentonite	Density (kg/m^3)	Liquid	Ref
C	$9.6 \cdot 10^{-12}$	$2.1 \cdot 10^{-11}$	Avonlea Na-bent	890	Saline GW	1
	$1 \cdot 10^{-11}$	$1.9 \cdot 10^{-11}$	Avonlea Na-bent	920	Saline GW	1
	$1.1 \cdot 10^{-11}$	$1.7 \cdot 10^{-11}$	Avonlea Na-bent	960	Saline GW	1
	$3 \cdot 10^{-12}$	$1.7 \cdot 10^{-11}$	Avonlea Na-bent	1180	Saline GW	1
	$8 \cdot 10^{-12}$	$1.7 \cdot 10^{-11}$	Avonlea Na-bent	1180	Saline GW	1
	$1.3 \cdot 10^{-12}$	$5.4 \cdot 10^{-12}$	Avonlea Na-bent	1250	Saline GW	1
Cl	$7.7 \cdot 10^{-12}$	$1.4 \cdot 10^{-10}$	Na-bent	1200	0.01 M NaCl	2
	$2.9 \cdot 10^{-11}$	$2 \cdot 10^{-10}$	Na-bent	1200	0.1 M NaCl	2
	$1.2 \cdot 10^{-10}$	$3.2 \cdot 10^{-10}$	Na-bent	1200	1 M NaCl	2
	$1.1 \cdot 10^{-11}$	$1.5 \cdot 10^{-10}$	Na-bent	1200	Saline GW	2
H	$1.5 \cdot 10^{-10}$	$1.1 \cdot 10^{-10}$	Ca-bent	1300	0.05 M CaCl$_2$	4
	$7.8 \cdot 10^{-11}$	$8 \cdot 10^{-11}$	Na-bent	1300	0.1 M NaCl	4
I	$9.4 \cdot 10^{-11}$	$7.6 \cdot 10^{-10}$	Avonlea Na-bent	900	Saline GW	3
	$3.3 \cdot 10^{-11}$	$1.05 \cdot 10^{-9}$	Avonlea Na-bent	920	Saline GW	3
	$4.6 \cdot 10^{-11}$	$6.4 \cdot 10^{-10}$	Avonlea Na-bent	1080	Saline GW	3
	$1.8 \cdot 10^{-11}$	$2.3 \cdot 10^{-10}$	Avonlea Na-bent	1090	Saline GW	3
	$2.7 \cdot 10^{-11}$	$2.5 \cdot 10^{-10}$	Avonlea Na-bent	1110	Saline GW	3
	$3.2 \cdot 10^{-11}$	$3.8 \cdot 10^{-10}$	Avonlea Na-bent	1290	Saline GW	3
	$2.9 \cdot 10^{-11}$	$1.6 \cdot 10^{-11}$	Ca-bent	1300	0.05 M CaCl$_2$	4
	$7.5 \cdot 10^{-12}$	$4.8 \cdot 10^{-11}$	Na-bent	1300	0.1 M NaCl	4
Sr	$1.5 \cdot 10^{-10}$	$1.8 \cdot 10^{-11}$	Ca-bent	1300	0.05 M CaCl$_2$	4
	$2.4 \cdot 10^{-11}$	$8.5 \cdot 10^{-12}$	Na-bent	1300	0.1 M NaCl	4
U	$2.1 \cdot 10^{-12}$	$8.4 \cdot 10^{-13}$	Na-bent (aerobic)	900	Saline GW	2
	$4.9 \cdot 10^{-13}$	$1.6 \cdot 10^{-12}$	Na-bent (aerobic)	1100	Saline GW	2
	$6 \cdot 10^{-14}$	$1.2 \cdot 10^{-13}$	Na-bent (aerobic)	1200	Saline GW	2
	$5.8 \cdot 10^{-12}$	$6.2 \cdot 10^{-13}$	Na-bent (aerobic)	1150	35000 ppm salt	5
	$5.7 \cdot 10^{-11}$	$7.5 \cdot 10^{-14}$	Na-bent (anaerobic)	1150	35000 ppm salt	5

1) Oscarson and Hume /1994/ in Yu and Neretnieks /1997/
2) Muurinen *et al*. /1989/ in Yu and Neretnieks /1997/
3) Oscarson *et al*. /1992/ in Yu and Neretnieks /1997/
4) Choi and Oscarson /1996/ in Yu and Neretnieks /1997/
5) Muurinen and Lehikoinen /1992/ in Yu and Neretnieks /1997/

Experimentally determined D_e-values are available for a few of the elements only, while D_a-values are reported for a larger number of elements. Therefore the D_a-values calculated from eq. 6-2 with density and porosity according to Table 6-10, K_d-values from Table 6-3 and $D_e = 1 \cdot 10^{-10}$ m^2/s are compared with experimentally determined D_a-values in Table 6-8 and in Figure 6-1.

Table 6-8. Comparison between calculated apparent diffusivity, D_a, and experimentally determined values of D_a for bentonite with a bulk density in the range 800 to 1300 kg/m^3

Element	D_a (m^2/s) calc.[a]	D_a (m^2/s) exp[b]	Bentonite	Density (kg/m^3)	Condition	Ref
C	$1.6 \cdot 10^{-10}$	$5.4 \cdot 10^{-12}$	Avonlea Na-bent	1250	Saline GW	1
		$6.5 \cdot 10^{-11}$		920		
Cl	$1.6 \cdot 10^{-10}$	$7.0 \cdot 10^{-11}$	Na-bent	1200	0.01 M NaCl	2
		$5.1 \cdot 10^{-10}$			1 M NaCl	
H	$1.6 \cdot 10^{-10}$	$8 \cdot 10^{-11}$	Na-bent	1300	0.1 M NaCl	4
		$1.1 \cdot 10^{-10}$	Ca-bent		0.05 M CaCl$_2$	
I	$1.6 \cdot 10^{-10}$	$1.8 \cdot 10^{-10}$	Avonlea Na-bent	1300	Saline GW	3
		$1.05 \cdot 10^{-9}$		920		
		$1.6 \cdot 10^{-11}$	Ca-bent	1300	0.05 M CaCl$_2$	4
		$4.8 \cdot 10^{-11}$	Na-bent	1300	0.1 M NaCl	
		$1.8 \cdot 10^{-10}$	Na (GEKO/QI)	1100	Concrete pH 13	6
Sr	$6.0 \cdot 10^{-11}$	$8.5 \cdot 10^{-12}$	Na-bent	1300	0.1 M NaCl	4
		$1.8 \cdot 10^{-11}$	Ca-bent		0.05 M CaCl$_2$	
		$2.3 \cdot 10^{-13}$	Na (GEKO/QI)	1100	Concrete pH 13	6
		$5.8 \cdot 10^{-12}$				
U	$9.0 \cdot 10^{-12}$	$1.2 \cdot 10^{-13}$	Na-bent (aerobic)	1200	Saline GW	2
		$3.8 \cdot 10^{-12}$		900		
		$7.5 \cdot 10^{-14}$	Na-bent (anaerob)	1150	35000 ppm salt	5
		$6.2 \cdot 10^{-13}$	Na-bent (aerobic)			
		$2.5 \cdot 10^{-13}$	Kunigel V1 Na-bent+ carbon steel	1200		7
		$4.4 \cdot 10^{-13}$		1000		
		$1.2 \cdot 10^{-12}$	Kunigel V1 Na-bent	1200		7
		$2.2 \cdot 10^{-12}$		1000		
		$8.8 \cdot 10^{-14}$	Kunipia F Na-bent + carbon steel	1200		7
		$2.2 \cdot 10^{-12}$		800		
		$3.3 \cdot 10^{-13}$	Kunipia F Na-bent	1200		7
		$3.7 \cdot 10^{-12}$		800		
Cs	$1.7 \cdot 10^{-11}$	$1 \cdot 10^{-11}$	Avonlea Na-bent	1250	Low+high saline	8
		$1.3 \cdot 10^{-11}$	Na (GEKO/QI)	1100	Concrete pH 13	6
Ni	$4.6 \cdot 10^{-12}$	$7.7 \cdot 10^{-13}$	Na (GEKO/QI)	1100	Concrete pH 13	6
		$9.6 \cdot 10^{-12}$				
Np	$9.5 \cdot 10^{-13}$	$5 \cdot 10^{-13}$	Kunigel V1 Na-bent	1000	90°C	9
		$2 \cdot 10^{-12}$			40°C	
		$1 \cdot 10^{-12}$	Na-bentonite	1200	Distilled water	10
		$5 \cdot 10^{-12}$		800		
Tc	$9.0 \cdot 10^{-12}$	$2.7 \cdot 10^{-12}$	Avonlea Na-bent reducing	1280	Saline GW	11
		$8.9 \cdot 10^{-12}$		1240		
		$1.7 \cdot 10^{-10}$	Avonlea Na-bent oxidising	1130	Saline GW	11
		$6.2 \cdot 10^{-10}$		940		

a) calculated from eq. 6.4.2 and porosity and density from Table 6-10, K_d from Table 6-3 and $D_e = 10^{-10}$ m^2/s

b) restricted to min and max values in the density range considered

1) Oscarson and Hume /1994/ in Yu and Neretnieks /1997/
2) Muurinen *et al.* /1989/ in Yu and Neretnieks /1997/
3) Oscarson *et al.* /1992/ in Yu and Neretnieks /1997/
4) Choi and Oscarson /1996/ in Yu and Neretnieks /1997/
5) Muurinen and Lehikoinen /1992/ in Yu and Neretnieks /1997/
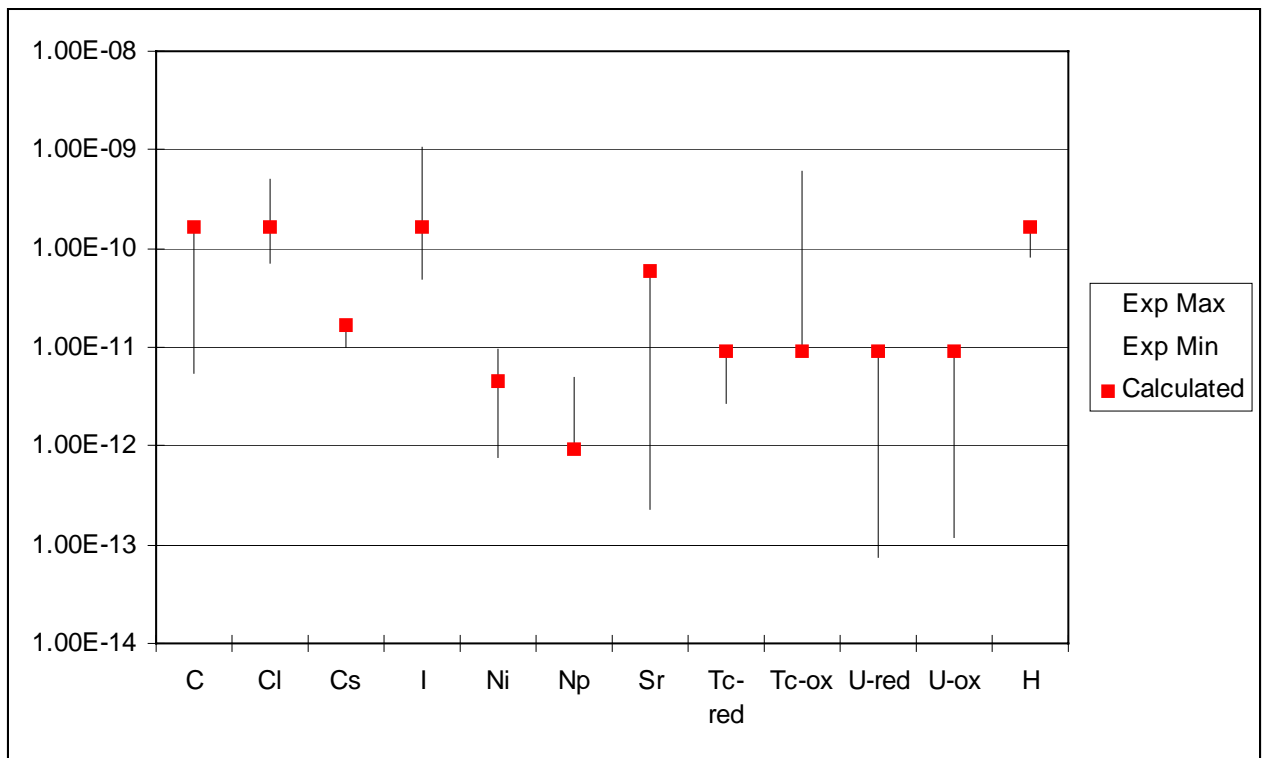6) Christiansen and Torstenfelt /1988/ in Yu and Neretnieks /1997/
7) Idemitsu *et al.* /1996/ in Yu and Neretnieks /1997/
8) Cheung /1989/ in Yu and Neretnieks /1997/
9) Tsukamoto *et al.* /1994/ in Yu and Neretnieks /1997/
10) Sato *et al.* /1992/ in Yu and Neretnieks /1997/
11) Sawatsky and Oscarson /1991/ in Yu and Neretnieks /1997/

Figure 6-1. *Maximum and minimum values of experimentally determined D_a (m^2/s) in bentonite with a density in the range 800 – 1300 kg/m^3 and D_a calculated from eq. 6-2.*

Experimentally determined D_a-values from experiments with deionised and distilled water are not included in Table 6-8 except for Np for which no other data are found. Figure 6-1 shows the whole range of experimentally determined D_a-values for each element and the D_a-value calculated from eq. 6-2. The figure indicates that the calculated D_a-value lies in the upper range of the experimentally determined values except for Tc under oxidising conditions and for Np, I and Cl. Since reducing conditions is expected the discrepancy with data for Tc under oxidising conditions can be disregarded. The experimental data for Np is scarce and those data reported are for conditions not really relevant for SFR (high temperature and Np(V), distilled water). Despite this, the difference between the measured maximum value and the calculated value is just a factor of 5.

For I and Cl it has already been shown in Table 6-7 that experimentally determined D_e-values in general are lower than 10^{-10} m^2/s. The fact that a D_a-value derived from a D_e-value of 10^{-10} m^2/s is lower than several of the experimentally determined D_a-values can be the result of the chosen value of the porosity. I and Cl are anions and due to anion exclusion effects the diffusion porosity for these anions can be smaller than the total porosity of the bentonite. Even if anion exclusion effects are expected to be smaller in saline water than in non-saline and in a bentonite with lower density, it is still probable that the porosity available for I and Cl diffusion in the Silo bentonite barrier is smaller than the total porosity. Neglecting this effect might underestimate the apparent diffusivity and thus the breakthrough time in the barrier. Since both [129]I and [36]Cl are long-lived nuclides this is of negligible importance. Furthermore, the diffusion flux through the barrier will not be underestimated since this is determined by the effective diffusivity, D_e.

In summary it is concluded that the experimental diffusion data available in the literature do not clearly call for a change in the previous assumption of an effective diffusivity of 10^{-10} m^2/s in the pure bentonite barrier in the Silo.

In regard to the D_e-value in the sand/bentonite barrier a similar comparison with experimental data as described above for bentonite has been made. However, the experimental data available in the literature are not that many. Uusheimo *et al*. /1993/ report experimentally determined D_e-values for Cl to be $3.7 \cdot 10^{-13}$ m^2/s and $6.9 \cdot 10^{-13}$ m^2/s in mixtures of 90 weight% tonalite and 10 weight% Na-bentonite. Higher D_e-values are measured for Cl in mixtures of 60 weight% granite and 40 weight% Na-bentonite, $1.3 \cdot 10^{-11}$ m^2/s and $1.6 \cdot 10^{-11}$ m^2/s /Uusheimo *et al*., 1993/.

Muurinen /1994/ reports results from measurements of sorption and diffusion of cesium and strontium in mixtures of sodium bentonite (10 weight%) and crushed rock (90 weight%). From experimentally determined values of D_a and K_d the effective diffusivity D_e is calculated to be of the order of 10^{-10} to 10^{-9} m^2/s for Cs and 10^{-10} to 10^{-8} m^2/s for Sr. In general the highest values of the effective diffusivity are calculated from results of experiments in water with a low salt content.

A D_e-value calculated from eq. 6-1 with a porosity of 25%, a diffusivity in unconfined water of $2 \cdot 10^{-9}$ m^2/s and neglecting any effects of constrictivity and tortuosity would give an effective diffusivity of $5 \cdot 10^{-10}$ m^2/s. In order to obtain an effective diffusivity of $1 \cdot 10^{-10}$ m^2/s the quotient between constrictivity and tortuosity (the geometric factor) has to be 0.2. This seems not to be an unrealistic value for a 90/10 sand bentonite mixture considering that a reasonable value of this quotient for a homogeneous porous material with distributed pore sizes is 0.1 /Höglund and Bengtsson, 1991/. Based on this and on the few data reported in the literature there is no reason to select any other value of the effective diffusivity D_e in the sand/bentonite barriers than the value of $1 \cdot 10^{-10}$ m^2/s that was assumed in the previous safety assessments of SFR.

In Table 6-9 values of the apparent diffusivity, D_a, calculated from eq. 6-2 with porosity and density according to Table 6-10, K_d from Table 6-4 and an effective diffusivity, D_e, of $1 \cdot 10^{-10}$ m^2/s are compared with experimentally determined values of D_a. For the elements Am, Np, U and Tc, the calculated value of D_a is lower than the mean value evaluated from experiments carried out by Albinsson and Engkvist /1989/. However, in the experiments Np, U, and Tc were all in a higher oxidation state than they are expected to be in the sand/bentonite barrier in the Silo. For other elements where experimentally evaluated D_a-values are available, these are in general lower than the value calculated from eq. 6-2. This could be seen in Table 6-9 and also in Figure 6-2. This comparison between experimentally determined D_a-values and D_a-values calculated assuming an effective diffusivity, D_e, of $1 \cdot 10^{-10}$ m^2/s gives no obvious reason to select another D_e-value than that used in the previous assessments of SFR. It is therefore decided to maintain the earlier assumed D_e-value of $1 \cdot 10^{-10}$ m^2/s.

Table 6-9. Comparison between calculated apparent diffusivity, D_a, and experimentally determined values of D_a for mixtures of rock/sand and bentonite.

Element	D_a (m²/s) calc.[a]	D_a (m²/s) exp[b]	Solid	Density (kg/m³)	Condition	Ref
Cl	$4 \cdot 10^{-10}$	$1.4 \cdot 10^{-10}$	90% tonalite		Groundwater	1
		$1.8 \cdot 10^{-10}$	10% Na-bentonite			
		$1.6 \cdot 10^{-10}$	60% granite		Groundwater	1
		$2.6 \cdot 10^{-10}$	40% Na-bentonite			
		$3.0 \cdot 10^{-10}$	90% sand	2000		2
			10% Na-bentonite			
I	$4 \cdot 10^{-10}$	$2 \cdot 10^{-11}$	90% sand	2000	Artificial GW	3
		$1.6 \cdot 10^{-10}$	10% Na-bentonite			
Cs	$4.9 \cdot 10^{-12}$	$5 \cdot 10^{-12}$	90% sand	2000	Artificial GW	3
			10% Na-bentonite			
		$6.5 \cdot 10^{-12}$	90% sand	2000	Saline GW (Äspö)	4
			10% Na-bentonite			
		$4.8 \cdot 10^{-13}$	90% rock		Groundwater ~200 ppm salt	5
			10% Na-bentonite			
		$4.5 \cdot 10^{-12}$	90% rock		Groundwater ~8000 ppm salt	5
			10% Na-bentonite			
		$3.4 \cdot 10^{-13}$	90% rock		NaCl, 0.001M	5
		$9.5 \cdot 10^{-12}$	10% Na-bentonite		NaCl, 0.5 M	
Sr	$1.5 \cdot 10^{-10}$	$4.6 \cdot 10^{-12}$	90% rock		Groundwater ~200 ppm salt	5
			10% Na-bentonite			
		$2 \cdot 10^{-11}$	90% rock		Groundwater ~8000 ppm salt	5
			10% Na-bentonite			
		$7.7 \cdot 10^{-12}$	90% rock		NaCl, 0.1M	5
		$1.5 \cdot 10^{-11}$	10% Na-bentonite		NaCl, 0.001 M	
Am	$5 \cdot 10^{-14}$	$3.2 \cdot 10^{-13}$	90% sand	2000	Artificial GW Am^{3+}	3
			10% Na-bentonite			
Pu	$5 \cdot 10^{-14}$	$< 1.6 \cdot 10^{-15}$	90% sand	2000	Artificial GW Pu^{4+}	3
			10% Na-bentonite			
Np	$5.6 \cdot 10^{-14}$	$4 \cdot 10^{-12}$	90% sand	2000	Artificial GW NpO_2^+	3
			10% Na-bentonite			
U	$5.6 \cdot 10^{-14}$	$1.6 \cdot 10^{-12}$	90% sand	2000	Artificial GW UO_2^{2+}	3
			10% Na-bentonite			
Tc	$1.7 \cdot 10^{-13}$	$3.2 \cdot 10^{-10}$	90% sand	2000	Artificial GW TcO_4^-	3
			10% Na-bentonite			

a) calculated from eq. 6.4.2 and porosity and density from Table 6-10, K_d from Table 6-4 and $D_e = 10^{-10}$ m²/s
b) restricted to min and max values where several data are available from the same experimental series
1) Uusheimo *et al.* /1993/ in Yu and Neretnieks /1997/
2) Johnston *et al.* /1984/ in Albinsson and Engkvist. /1989/
3) Albinsson and Engkvist /1989/
4) Albinsson /1993/ in Wanner *et al.* /1994/
5) Muurinen /1994/ Appendix II
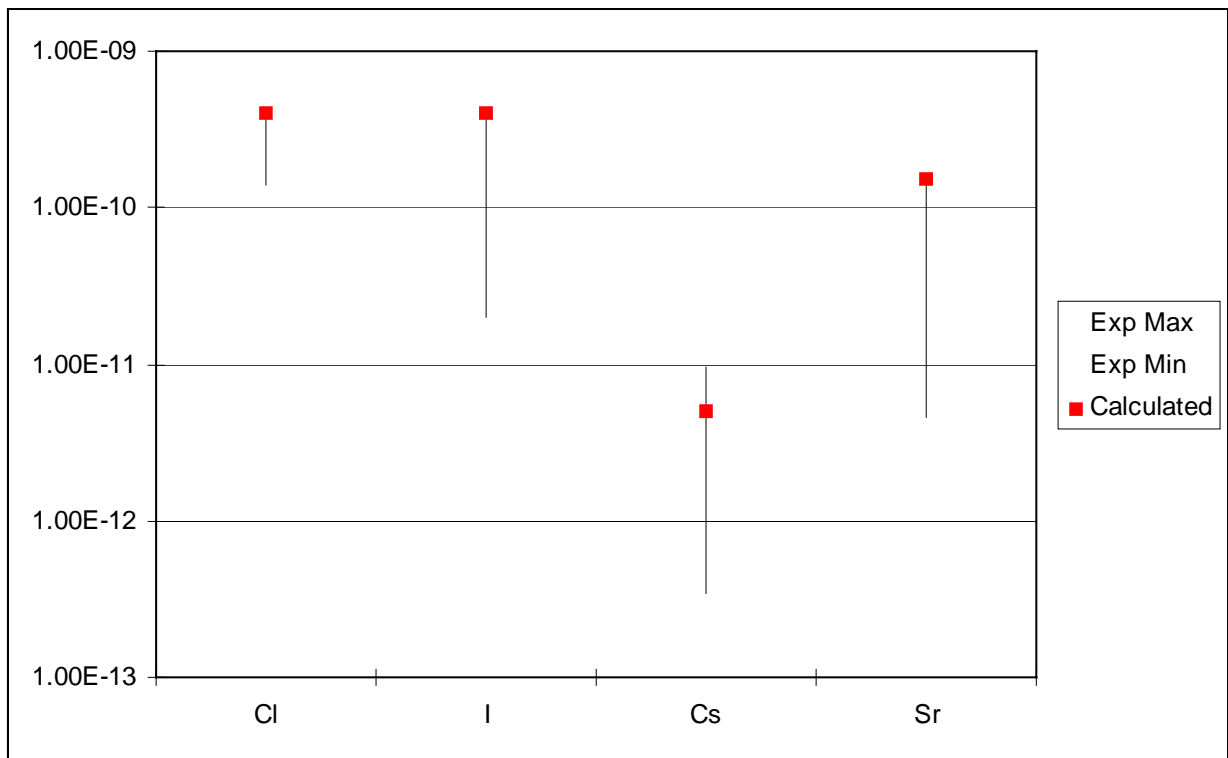
Figure 6-2. Maximum and minimum values of experimentally determined D_a (m^2/s) in mixtures of sand or rock and bentonite and D_a calculated from eq. 6-2.

Rock fill

The rock fill that will be used in SFR is here assumed to be similar to the sand/gravel fill defined for the SFL 3-5 repository concept. In the preliminary safety assessment of SFL 3-5 a porosity of 30% was selected for the fill and the effective diffusivity, D_e, was set to $6 \cdot 10^{-10}$ m^2/s, neglecting any affects of constrictivity and tortuosity of the pores in the fill /Skagius *et al.*, 1999/. By assuming a solid density of the material of 2700 kg/m^3, the bulk density can be calculated to 1890 kg/m^3 for the dry material.

6.4.3   Selected data

In Table 6-10 the selected values on effective diffusivity, porosity and bulk density for the different engineered barriers in SFR are compiled. The background to the selected data is given in the previous subsection.

Table 6-10. Values of the effective diffusivity, porosity and bulk density selected for the engineered barrier materials.

Material	Effective diffusivity (m^2/s)	Porosity (m^3/m^3)	Bulk density (kg/m^3)
Structural concrete	$1 \cdot 10^{-11}$	0.15	2300
Concrete grout in Silo	$1 \cdot 10^{-10}$	0.30	2000
Concrete grout in BTF	$1 \cdot 10^{-10}$	0.20	2300
Bentonite	$1 \cdot 10^{-10}$	0.61	1050
Sand/bentonite 90/10	$1 \cdot 10^{-10}$	0.25	2000
Rock fill (sand/gravel)	$6 \cdot 10^{-10}$	0.30	1890

6.4.4 Uncertainties

The uncertainty associated with the selected values of porosity and effective diffusivity in the engineered barrier materials has to some extent already been addressed in Section 6.4.2. These uncertainties can be summarised as follows.

Concrete

The porosity of fresh structural concrete is about 10%. Due to chemical alteration in contact with groundwater the porosity will change. Over a time period of 10 000 years the porosity is expected to be in the range 7 to 19% depending both on time and on distance from the concrete-groundwater interface /Höglund, 2001/. This should be compared with the selected porosity of 15% for the whole time period of 10 000 years.

The selected effective diffusivity of $1 \cdot 10^{-11}$ m^2/s is representative for fresh structural concrete /Skagius et al., 1999/. Due to chemical alteration the diffusivity may change mainly in those parts that are substantially depleted of CSH phases. Theoretically the diffusivity could be of the order of 10 times higher in such parts of the concrete. However, extensive depletion of CSH will only occur in the outermost few centimetres of the concrete structures in BMA and BTF within 1000 years and in the outermost 0.2 m after 10 000 years. For BMA with the thinnest walls (0.4 m) the effect of neglecting this possible increase in diffusivity is that the steady-state diffusion flux is underestimated with at most about 10% after 1000 years and with at most a factor of 2 after 10 000 years.

The porosity of the Silo and BTF concrete grout is selected based on calculations with a hydration model using the actual mixing proportions. The effective diffusivity is selected as being 10 times higher than in structural concrete because of a larger capillary porosity. There are no experimental data available on diffusivity in these types of concrete grout so it is difficult to assess the uncertainty in the selected value. However, the effective diffusivity of K, Ca and NO$_3$ has been evaluated from leaching experiments on a high porosity cement mortar of similar type as the SFR grout (w/c ratio 0.7 and 0.9) /Section 6 in Adenot et al., 2001/. The effective diffusivity evaluated from 90 days of leaching are $8.2 \cdot 10^{-11}$ m^2/s for K and $1.5 \cdot 10^{-13}$ m^2/s for Ca. For NO$_3$ the effective diffusivity was evaluated to be $3.7 \cdot 10^{-11}$ m^2/s assuming that all NO$_3$ is dissolved in the porewater and $8.1 \cdot 10^{-11}$ m^2/s with the assumption that a fraction of the NO$_3$ is bound in the minerals in the cement. The values derived for K and NO$_3$ are slightly lower than the selected value of $1 \cdot 10^{-10}$ m^2/s, while the value derived for Ca are significantly lower. Neither the Silo grout nor the BTF grout is expected to be exposed to any significant depletion of CSH phases during a time period of 10 000 years. Therefore, no dramatic changes in the porosity and effective diffusivity with time are expected.

Bentonite and sand/bentonite

The uncertainty in the selected values of effective diffusivity in bentonite and mixture of sand and bentonite is to some extent reflected in the tables and figures in Section 6.2.3 where the selected values are compared with experimentally derived values. For bentonite, the comparison is restricted to experimental data from experiments in saline water. This means that ion exclusion should have little effect on the diffusion of anions and that "surface diffusion" of cations should be depressed. Surface diffusion here refers to the observed higher mobility in clays and micropores in rock of cations like Cs and Sr in water with low ionic strength as compared to in water with high ionic strength (see e.g. Yu and Neretnieks /1997/ and Ohlsson /2000/). The

future expected change in groundwater composition to less saline water could make ion exclusion and surface diffusion more important.

The effect of ion exclusion would be a decrease in diffusion porosity for the anions and thus also a decrease in effective diffusivity. Based on experimental data Muurinen *et al*. /1994/ has given an expression for the dependence of effective and apparent diffusivity on bentonite density for Cl diffusion at a water salinity of 0.013 M NaCl (about 750 ppm salt). From that expression the effective diffusivity D_e is about $1.4 \cdot 10^{-11}$ m^2/s and D_a is about $2.4 \cdot 10^{-10}$ m^2/s. These diffusion values would correspond to an effective porosity for Cl of about 6% (eq. 6-2). These values should be compared to the selected $D_e = 1 \cdot 10^{-10}$ m^2/s and porosity = 61% and the calculated $D_a = 1.6 \cdot 10^{-10}$ m^2/s. In sand/bentonite mixtures the bentonite is dilute and the effect of ion-exclusion should be small.

Surface diffusion, on the other hand, would mean an increased diffusion rate of cations like Sr and Cs when the water becomes less saline. Since ^{90}Sr is a short-lived radio-nuclide it will have decayed before the salinity of the water decreases. The same situation will apply for ^{137}Cs. For the more long-lived ^{135}Cs it cannot be excluded that surface diffusion effects may become important at times longer than 1000 years after repository closure when the water becomes less saline. Based on diffusion experiments in compacted bentonite, Eriksen and Janson /1996/ has showed that both D_a and D_e values for Cs and Sr vary with K_d as this change with the ionic strength of the solution. For bentonite with a density of 1800 kg/m^3 and a solution corresponding to a non-saline groundwater (ionic strength = 0.018 mol/dm^3), D_e was evaluated to be $6.4 \cdot 10^{-10}$ m^2/s and D_a to be $1 \cdot 10^{-12}$ m^2/s for Cs. From experiments with Na-bentonite with a density of 1000 kg/m^3 and distilled water Sato *et al*. /1992/ give D_a for Cs to be $4.8 \cdot 10^{-12}$ m^2/s. A similar value of $D_a = 4.8 \cdot 10^{-12}$ m^2/s is reported by Miyahara *et al* /1991/ for Cs diffusion in Kunipia F Na-bentonite in distilled water. These results indicate that the selected D_e-value of $1 \cdot 10^{-10}$ m^2/s might be somewhat low when the groundwater has become less saline while the calculated D_a-value of $1.7 \cdot 10^{-11}$ m^2/s still is higher than the experimentally determined values.

Surface diffusion effects might also be relevant for Cs in the sand/bentonite barriers as the salinity of the water decreases. There are no experimentally determined D_e-values available that can give an indication on the effect. The comparison between D_a calculated from the selected values of D_e, porosity and K_d given in Table 6-9 and in Figure 6-2 shows that the calculated D_a data is lower than experimentally determined D_a in low-saline water.

Due to chemical interaction with components leached from the cement and with species in the groundwater the mineralogical composition and the porosity of the bentonite and sand/bentonite may change. This may in turn affect the diffusivity in these materials. The hydrogeochemical modelling carried out by Höglund /2001/ showed a decrease in the porosity of the sand/bentonite barrier from an initial porosity of 25% to a minimum value of about 19% close to the interface between concrete and sand/bentonite. This modelling did not take into account the dissolution of minerals in the sand/bentonite such as montmorillonite, quartz etc., but a recent modelling of a similar system where dissolution of the primary minerals are considered shows similar results /Savage *et al*., 2001/. Based on their results, Savage *et al* /2001/ conclude that hyperalkaline fluids may cause extensive alteration of the chemical and physical properties of bentonite by dissolving silicate and aluminosilicate minerals which are replaced by secondary minerals such as calcium silicate hydrates (CSH), zeolites and sheet silicates. However, the growth of these secondary solids will in most cases lead to a complete filling of the

available pore space close to the cement-bentonite interface over time-scales of the order of 100 to 1000 years /Savage *et al*., 2001/. These results indicate that the effects of a potential future alteration of the bentonite and sand/bentonite barriers rather should be towards a more effective diffusion barrier than the opposite. By not considering these potential changes, the diffusive release of radionuclides should not be underestimated.

Rock fill

The porosity of gravel is expected to be in the range 25 – 40% and here the rock fill is assigned a porosity of 30%. The selected value of the effective diffusivity is based on this porosity and neglecting any effects of constrictivity and tortuosity. The selected value of the porosity can be somewhat low, but should well be balanced by the omission of the effects of pore structure. Due to impact of concrete porewater, calcite and brucite may precipitate in the pore space and calcium silicate hydrates that potentially form at the surface of the solid material may lead to volume changes and reduction in porosity. By disregarding such possible effects, the diffusive transport of radionuclides in the rock fill is not underestimated.

7 Migration data – geosphere

7.1 Flow related migration parameters

7.1.1 Data needed

Far field migration essentially depends on the velocity of the water and the strength of the interaction between the flowing water and the rock matrix. The former essentially determines the breakthrough time of non-reactive solutes, and the latter essentially controls the retardation of solutes by diffusion into the rock matrix and sorption onto mineral surfaces. The current SKB migration code FARF31 needs travel time and flow wetted surface per volume of water and the Peclet-number. The interaction between flowing water and rock matrix is controlled by the F-value (see e.g. /Andersson *et al*., 1998/). Formally $F = t_w a_w$, but a_w only has a clear interpretation when flow and porosity are constant along migration paths. When selecting values of a_w one needs to understand that t_w and a_w are strongly related. The a_w-value to select for FARF31 should be the one that produces the right F value.

Generally, travel time and accumulated F-values along a migration path are given by, see e.g. /Andersson *et al*., 1998/:

$$t_{w,i} = \{\int \varepsilon_f(s)/q(s)ds\}_i, \qquad\qquad (7\text{-}1)$$

$$F_{tot,i} = \{\int a_r(s)/q(s)ds\}_i) \qquad\qquad (7\text{-}2)$$

where a_r (m^{-1}) is the local flow wetted surface per volume of rock. Locally, a_w and a_r are related by

$$a_w = a_r/\varepsilon_f \qquad\qquad (7\text{-}3)$$

If porosity and flow are constant this means that $t_w = L\varepsilon_f/q$ and $F = a_r L/q$ (independent of porosity), where q is the groundwater flux (Darcy velocity).

The biosphere analyses needs information on discharge areas.

7.1.2 Source of data

Based on the flow situation at different distinct times, Holmén and Stigsson /2001a/ calculates travel times both for varying flow porosity, t_w, and for a constant flow porosity of 0.01, $t_{0.01}$. These results may be used to estimate travel time and F-parameter to be used in the migration calculations.

The travel time calculations using a variable flow porosity ε_f between 0.5% (in rock mass) and between 1% - 5% in fracture zones are direct estimates of the travel time distribution to use in the migration calculations. These travel times cannot be used to estimate the transport resistance, F, as this depends on the integrated inverse of the flow rather than on the integrated inverse of velocity. However, using travel times calculated with constant porosity $t_{0.01}$ and assuming a constant flow wetted surface a_r, equation 7-2 shows that:

$$F = a_r t_{0.01}/0.01 = 100 a_r t_{0.01} \qquad\qquad (7\text{-}4)$$

There are no estimates of the a_r at SFR. Based on values used in SKB SR 97 it may be assumed that the flow wetted surface per volume of rock a_r is in the order of 1 m^{-1} /Andersson *et al.*, 1998/. This means that $F=100t_{0.01}$.

Table 7-1 displays 10th and 50th percentiles of the F-parameter (year/m) assuming $a_r=1$ m^{-1} and 50th percentiles of the migration time t_w (year) according to Holmén and Stigsson /2001a/. The F-values suggest that at least some nuclides will be significantly retarded in the far-field geosphere.

Table 7-1. Median travel time (t_w) and 10th and 50th percentiles of the F-parameter (year/m) assuming $F=100t_{0.01}$, where $t_{0.01}$ is taken from tables 11.8-11-15 and t_w is taken from tables 11.1- 11.7 of Holmén and Stigsson /2001a/.

Time	BLA			BTF1			BTF2			BMA			Silo		
AD	$t_{w,50}$	F_{50}	F_{10}	$t_{w,50}$	F_{50}	F_{10}	$t_{w,50}$	F_{50}	F_{10}	$t_{w,50}$	F_{50}	F_{10}	$t_{w,50}$	F_{50}	F_{10}
2000	56	2300	1300	58	2300	1900	56	2300	2000	248	$5 \cdot 10^4$	6800	313	$6 \cdot 10^4$	$6 \cdot 10^4$
3000	18	1300	900	119	$2 \cdot 10^4$	9100	44	6400	2300	52	9300	1500	379	$3 \cdot 10^4$	$1 \cdot 10^4$
4000	87	3300	1300	384	$4 \cdot 10^4$	9800	214	9600	6000	74	5500	2200	121	9100	7800
5000	127	4400	2200	491	$6 \cdot 10^4$	$1 \cdot 10^4$	286	$2 \cdot 10^4$	6800	84	5900	2600	129	$1 \cdot 10^4$	8500
6000	137	4600	2400	521	$6 \cdot 10^4$	$1 \cdot 10^4$	297	$2 \cdot 10^4$	7200	86	5800	2700	131	$1 \cdot 10^4$	8800
7000	137	4600	2300	521	$6 \cdot 10^4$	$1 \cdot 10^4$	303	$2 \cdot 10^4$	7100	87	5900	2700	131	$1 \cdot 10^4$	8800

7.1.3 Evaluation of data and uncertainties

Travel time and flow wetted surface

One could clearly argue that the porosity values used by Holmén and Stigsson are high in relation to what is usually considered in crystalline rock, see e.g. Andersson *et al.*, /1998/. The basis for selection such high porosity values is that smaller values would imply a fast breakthrough of Baltic water into the vaults. Such a breakthrough has not yet been observed. Considering that the values could represent crushed rock etc. they are not unrealistic. Still, it is evident that the present selection of values may over-estimate the retention of non-sorbing elements. However, for sorbing elements retention is governed both by the travel time and the "F-factor". The latter does not depend on flow porosity!

According to results in Table 7-1 there are some differences in travel time and transport resistance between the vaults. After 3000 AD the longest time is from BTF1 and the shortest from BMA. The transport resistance is largest from BTF1 and smallest from BLA. Potentially, there may also be different travel times for releases occurring in different sections of the vaults. However, considering the uncertainties and the fact that most path lines go through the intersecting fracture zones (true for the horizontal repository vaults) or enters the rock quite uniformly (true for the Silo) it is not judged worthwhile to attach different far-field migration characteristics to different part of the vaults. For each vault all near-field releases will be assumed to enter one "far-field". The differences between vaults may still be upheld.

There is variability in the calculated transport resistance, but the difference between the 10th and the 50th percentiles in Table 7-1 is only about a factor of 4 and sometimes less. It is likely that these differences are small in relation to the unresolved small-scale variability of the flow field and the uncertainty in a_r. In addition, as will be explained below the presence of colloids cold not be excluded. All these uncertainties (and variability) will be handled by analysing a case with no retention in the far field.

The migration paths, t_w and F changes with time due to the shoreline displacement. In general retention is less during the period 2000 AD to 4000 AD, i.e. the times of most interest. The far field migration code could not handle this directly. Instead the following procedure is suggested.

- Migration end points will always be assumed to occur at the points predicted by the groundwater pathway analysis of Holmén and Stigsson /2001a/. This defines which type of biosphere to which there may be radionuclide releases from the SFR.

- The change of migration paths in the rock over time will not be explicitly considered. Instead different cases with constant migration properties in FARF31 will be analysed. The cases should cover the uncertainty range.

- A "reasonable" case is to select "median" values of t_w and F (with associated a_w) for each vault to represent migration conditions for the period 2000 AD to 4000 AD. For longer times these values are too pessimistic, but will be used anyway for convenience.

- A clearly pessimistic case is to assume no retention at all in the rock, but still use the (above) release points (discharge areas) given by the far-field path lines.

Table 7-2 shows the resulting data based on these suggestions. It should also be noted that the SKB migration code FARF31 requires t_w and a_w as input, whereas the predicted migration parameters are given in terms of t_w and F. In order to provide the correct F values the a_w should simply be selected by let $a_w = F/t_w$.

Table 7-2. Representative far-field retention data for the different vaults, where a_w is calculated as $a_w = F/t_w$ (t_w in years and a_w in m^{-1}).

Case	BLA			BTF1			BTF2			BMA			Silo		
	t_w,	F	a_w	t_w,	F	a_w	t_w,	F	a_w	t_w,	F	a_w	t_w,	F	a_w
Reason.	50	2000	40	100	$2 \cdot 10^4$	200	50	6000	120	50	6000	120	300	$3 \cdot 10^4$	100
Pess.	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

The similarity in the values suggested in Table 7-2 for the reasonable case indicates that there is no obvious reason to assume different values for the different repository parts. Therefore it is decided to use the same value for all repository parts and the following values is selected:

$$t_w = 50$$

$$F = 6000$$

$$a_w = 120$$

These values are the same as those suggested in Table 7-2 for 2BTF and BMA, but more pessimistic than those suggested for 1BTF and the Silo. For BLA the selected reasonable values will somewhat overestimate the retention in the rock.

Peclet numbers

Andersson *et al.* /1998/ conclude that the importance of "Peclet" numbers in FARF31 is secondary to other parameters. They also note that literature data fall within the range 2 to 40 /Elert *et al.* 1992/. Based on this it is suggested to use a Peclet number 10 as a *reasonable estimate* and a range of 2 - 50. These values are generic rather than site specific.

7.1.4 Selected data

Table 7-3 summarises the selected far-field, flow-related migration data.

Table 7-3. Suggested far-field, flow-related migration data

Case	t_w (year)	a_w (m^{-1})	(F-value)	Pe
Realistic	50	120		10
Pessimistic	0	0	0	n.a.

7.2 Sorption and diffusion in the rock matrix

7.2.1 Data needed

In addition to flow-related migration data, the model for calculating radionuclide migration in the geosphere needs data on the porosity of the rock matrix, the diffusivity in the pores of the rock matrix, the maximum penetration depth into the rock matrix by matrix diffusion and the sorption distribution coefficients, K_d, for radionuclides in the rock.

7.2.2 Source of data

The values of the parameters describing sorption and diffusion in the rock matrix are primarily taken from the recent safety assessment of a deep repository for spent fuel, SR 97 /SKB, 1999a and Andersson, 1999/. For elements of importance in the SFR waste and not included in the data derived within SR 97, parameter values are taken from the preliminary assessment of the SFL 3-5 repository concept /SKB, 1999b and Skagius *et al.*, 1999/.

7.2.3 Evaluation of data and uncertainties

Matrix porosity

The porosity of the rock matrix available for diffusion of radionuclides is for Swedish rock of the order of 0.1 to 1% /Ohlsson and Neretnieks, 1997/. A rock matrix porosity of 0.5% was used both in SR 97 and in the preliminary assessment of SFL 3-5. This value is also selected for the radionuclide migration calculations within SAFE.

The present groundwater in SFR is saline and anion exclusion and thus a smaller effective porosity for anion diffusion is discarded even if anion exclusion effects has been noticed in solutions with as high ionic strength as 0.2 M /Ohlsson, 2000/. The future change towards a less saline groundwater would imply a smaller effective porosity of anions like I and Cl and inorganic C. In the preliminary assessment of SFL 3-5 an effective porosity of 0.05% was assumed for anions in non-saline water /Skagius *et al.*, 1999/. This potential reduction in diffusion porosity at longer times (more than 1000 years after repository closure) is not considered in the migration calculations within SAFE. This would mean that the retardation of anions is overestimated at longer times. However, this uncertainty and other uncertainties regarding matrix porosity, e.g. in spatial variability, that would give rise to higher release rates of nuclides than with the selected value are covered by the pessimistic case calculations where no retention at all in the geosphere is considered.

Penetration depth

The maximum penetration depth into the rock matrix depends on the structure of the rock in terms of connected porosity. The uncertainty in this parameter is large, but an

estimate can be made from the symmetry limit that diffusion cannot proceed deeper into the rock than half the distance between two active migration paths and from values of the flow-wetted surface per volume of rock. For a flow-wetted surface area of 1 m^2 per m^3 rock, the maximum penetration depth is 2 m. This value was used in SR 97 and is also selected for the migration calculations within SAFE. This parameter is not very important since the actual penetration depth for a non-sorbing radionuclide is of the order of 1 to 2 dm for a travel time of the order of 50 years and much shorter for a sorbing nuclide.

Matrix diffusivity

Values of the effective diffusivity in the rock matrix are selected to be the same as those that were selected for the preliminary assessment of SFL 3-5 /Skagius *et al.*, 1999/. The selected values are compiled in Table 7-5. The values are element specific and representative for saline groundwater. Most of the values were originally proposed by Ohlsson and Neretnieks /1997/ as reasonable values for the use in SR 97, but for the preliminary assessment of SFL 3-5 additional values had to be chosen for elements not considered by Ohlsson and Neretnieks. How these additional values were chosen is described in Skagius *et al.* /1999/.

Effects of anion exclusion and surface diffusion of cations, which would become important at longer times when the groundwater will be less saline than the present groundwater, is not considered. Neglecting surface diffusion of cations implies that the diffusion into the rock matrix and thereby the retention in the rock of these cations is underestimated. Neglecting anion exclusion has the opposite effect, i.e. the retention in the rock of anions is overestimated. However, the uncertainty introduced by neglecting this effect as well as other uncertainties associated with the selected values of effective diffusivity that could lead to higher release rates are covered by the analysis of the pessimistic case with no retention at all in the geosphere.

Sorption

The selected values of the sorption coefficient K_d (see Table 7-5) are taken from the set of data chosen as reasonable values in saline groundwater in SR 97 /Andersson, 1999/. The same data set was used in the preliminary assessment of SFL 3-5 with the addition of some values for elements that were not relevant in SR 97. The selection of these additional data is described in Skagius *et al.* /1999/.

The original data set used in SR 97 was proposed by Carbol and Engkvist /1997/ in terms of a reasonable value and an uncertainty interval for each element. The data are representative for saline water, pH > 7 and reducing conditions (Eh < -200 mV). The uncertainty interval given by Carbol and Engkvist is based on the scattering of experimental data reported in the literature.

Some of the elements are sensitive to the ionic strength of the water, e.g. Cs and Sr, and other elements are sensitive to redox conditions, e.g. Tc and Np. The impact of a future change to a less saline groundwater would be a higher sorption of elements like Sr and Cs. This is not relevant for ^{90}Sr and ^{137}Cs because of the short half-life in comparison with the predicted time of at least 1000 years before less saline groundwater conditions are established. For ^{135}Cs the omission of the potentially higher sorption in the future will overestimate the release.

The selection of K_d-values representative for reducing conditions may be uncertain at least in the rock close to the biosphere boundary. Other uncertainties are associated with the content of organic compounds in the water that could affect sorption. However,

these uncertainties and other uncertainties associated with the selected values of K_d that would give rise to higher release rates of nuclides than with the selected values are covered by the pessimistic case calculations where no retention at all in the geosphere is considered.

7.2.4 Data selected

The selected values of rock matrix porosity, maximum penetration depth into the rock matrix by diffusion, element specific D_e and K_d are compiled in this subsection. The background to the selected data is given in the previous subsection.

Table 7-4. Selected values of rock matrix porosity and maximum penetration depth into the rock matrix by diffusion.

Parameter	
Matrix porosity, ε (m^3/m^3)	0.005
Maximum penetration depth, x_0 (m)	2

Table 7-5. Selected values of element specific effective diffusivity, D_e, and sorption coefficient, K_d for saline groundwater /Skagius et al., 1999/.

Element	D_e (m^2/s)	K_d (m^3/kg)
H	$1.0 \cdot 10^{-13}$	0
C inorg	$5.0 \cdot 10^{-14}$	0.001
C org	$4.0 \cdot 10^{-14}$	0
Cl	$8.3 \cdot 10^{-14}$	0
Co	$2.9 \cdot 10^{-14}$	0.02
Ni	$2.8 \cdot 10^{-14}$	0.02
Se	$4.0 \cdot 10^{-14}$	0.001
Sr	$3.3 \cdot 10^{-14}$	0.0002
Zr	$4.0 \cdot 10^{-14}$	1
Nb	$4.0 \cdot 10^{-14}$	1
Mo	$4.0 \cdot 10^{-14}$	0
Tc(IV)	$4.0 \cdot 10^{-14}$	1
Pd	$4.0 \cdot 10^{-14}$	0.01
Ag	$7.1 \cdot 10^{-14}$	0.05
Cd	$3.0 \cdot 10^{-14}$	0.02
Sn	$4.0 \cdot 10^{-14}$	0.001
I	$8.3 \cdot 10^{-14}$	0
Cs	$8.8 \cdot 10^{-14}$	0.05
Sm	$4.0 \cdot 10^{-14}$	2
Eu	$4.0 \cdot 10^{-14}$	2
Ho	$4.0 \cdot 10^{-14}$	2
U(IV)	$4.0 \cdot 10^{-14}$	5
Np(IV)	$4.0 \cdot 10^{-14}$	5
Pu	$4.0 \cdot 10^{-14}$	5
Am	$4.0 \cdot 10^{-14}$	3
Cm	$4.0 \cdot 10^{-14}$	3

8 Biosphere

8.1 General

In this chapter the data used as input to the biosphere model system are defined. In order to include uncertainties concerning the evolution of the biosphere in the SFR-area a number of cases have been set up and modelled. One case was set up to describe the most reasonable evolution of the area, i.e. first a coastal bay that becomes a lake and later is drained and used as agricultural land. Alternative cases are a well case, a mire case and a case where the conditions today are assumed to prevail during 10 000 years.

The model system set up for the reasonable case consists of four models:

- a coastal model describing the conditions today (Coast 1, used for the time period 2000 AD – 4000 AD)

- a coastal model with smaller water volumes and larger retention times (Coast 2, used for the time period 4000 AD – 5000 AD)

- followed by a lake model (5000 AD – 8000 AD), and finally

- an agricultural land model (8000 AD – 12000 AD).

Radionuclides accumulated in the sediments during the coastal and lake stages are included as an initial inventory in the soil in the agricultural land model. The models used for the other cases are a well model (for the time period 4000 AD – 12000 AD), a mire model (4000 AD – 12000 AD) and a coastal model (Coast 3, 2000 AD – 12000 AD). For these models constant biosphere conditions are assumed during the simulated time periods. The models are described in detail in Karlsson *et al* /2001a/ whereas the evolution of the biosphere in the area is described in Kautsky /2001/ and in the main safety report /SKB, 2001a/.

The parameters used in the biosphere models can be divided into five sets according to their properties. Geometrical and physical/chemical parameters are used to calculate the dispersion of radionuclides in and between different parts of the modelled system. Biological and radiological parameters as well as those describing living habits of humans and cattle are used when calculating the exposure to man.

- *Geometrical parameters* (areas, depths etc of the different physical components)

- *Physical/chemical parameters* (water flows, sorption parameters etc.)

- *Biological parameters* (root uptake, uptake to fish, crustacean and aquatic plants, translocation, metabolism in cattle etc.)

- *Living habits of humans and cattle* (irrigation, keeping cattle outdoors, consumption patterns etc.)

- *Radiological parameters (*dose conversion factors, half-lives of radionuclides)

The model system performs probabilistic calculations, which means that input parameter values are given as best estimate, minimum and maximum values and type of distribution. The probabilistic approach enables uncertainties and variations, two

prevailing aspects when dealing with biosphere parameters, to be considered. Often, information on real type of distribution for a specific parameter is lacking because of scarcity of data. In these cases the parameters have been given triangular (for narrow ranges) or log-triangular distributions (for ranges over orders of magnitudes), as is recommended by IAEA /1995/. Log-triangular distributions are also used for parameters with skewed distributions.

The input of radionuclides to the different models is calculated release rates (Bq/year) as a function of time from the far field (geosphere). This source of radionuclides is introduced in the biosphere models as contaminated groundwater. It is considered that it reaches the recipient without any influence of sorption or retention when the ground-water passes from geosphere to biosphere conditions (reductive environment, low organic content versus oxidative conditions and higher organic content and biological activity). This is conservative in that all radionuclides reaches the biosphere without any retention in sediments whereas it may be non-conservative with respect to the exposure to radionuclides retained in the sediments.

8.2 Data needed

In short the models use the following parameters.

8.2.1 Coastal models (Coast 1, 2 and 3)

- *Geometrical parameters* (water areas, mean depths, the fraction of accumulation bottoms and the depth of the upper sediments of the three parts of the models; the Model area, Öregrundsgrepen and the Baltic Sea).

- *Physical/chemical parameters* (water retention times, sediment growth rate, suspended matter and fine particle settling velocity, distribution coefficients for partition of radionuclides between water and suspended matter in brackish water).

- *Biological parameters* (uptake to fish, crustacean and aquatic plants as well as metabolism in cattle).

- *Living habits of humans and cattle* (consumption patterns for humans and cattle and time for keeping cattle at the shoreline).

- *Radiological parameters (*dose conversion factors, half-lives of radionuclides).

8.2.2 Lake model

- *Geometrical parameters:* area, depth, the fraction of accumulation bottoms and the depth of the upper sediments of the lake, area, depths and porosity of different soil layers of garden plot irrigated with lake water.

- *Physical/chemical parameters*: water retention time, sediment growth rate, suspended matter and fine particle settling velocity, water transport between different soil layers, soil density and erosion, bioturbation, retention of radionuclides on vegetation surfaces, weathering half-life and dust concentration in air, distribution coefficients for partition of radionuclides between water and solid matter in soil and lake water.

- *Biological parameters*: uptake to fish, crustacean and aquatic plants, root uptake, translocation, metabolism in cattle, yield values.

- *Living habits of humans and cattle*: consumption patterns for humans and cattle, staying outdoors, inhalation rate, irrigation, keeping cattle at shoreline.

- *Radiological parameters:* dose conversion factors, half-lives of radionuclides.

8.2.3　Agricultural land model

- *Geometrical parameters:* field area, depth and porosity of different soil layers.

- *Physical/chemical parameters*: water transport between different soil layers, soil density and erosion, bioturbation, dust concentration in air, distribution coefficients for partition of radionuclides between water and solid matter in soil.

- *Biological parameters*: root uptake, metabolism in cattle.

- *Living habits of humans and cattle*: consumption patterns, staying outdoors, inhalation rates, keeping cattle outdoors, yield values.

- *Radiological parameters:* dose conversion factors, half-lives of radionuclides.

8.2.4　Mire model

- *Geometrical parameters:* area, depth and porosity of the peat.

- *Physical/chemical parameters*: runoff, density and dust concentration in air, distribution coefficients for partition of radionuclides between water and solid matter in soil.

- *Biological parameters*: root uptake, metabolism in cattle.

- *Living habits of humans and cattle*: consumption patterns for humans and cattle, staying outdoors, inhalation rate, keeping cattle outdoors, yield values, fuel load.

- *Radiological parameters:* dose conversion factors, half-lives of radionuclides.

8.2.5　Well model

- *Geometrical parameters:* area, depth and porosity of different soil layers of the irrigated garden plot.

- *Physical/chemical parameters*: dilution volume of the well, water transport between different soil layers, soil density and erosion, bioturbation, retention of radionuclides on vegetation surfaces, weathering half-life and dust concentration in air, distribution coefficients for partition of radionuclides between water and solid matter in soil.

- *Biological parameters*: root uptake, translocation, metabolism in cattle.

- *Living habits of humans and cattle*: consumption patterns for humans and cattle, staying outdoors, irrigation, yield values.

- *Radiological parameters:* dose conversion factors, half-lives of radionuclides.

8.3 Source of data

When estimating data for *geometrical parameters* investigations at the site as well as model prognoses for the site have been used. This is also true for some *physical/chemical parameters* such as water retention times whereas data about e.g. suspended matter, fine particle sinking velocity, water transport in soil layers, soil density and porosity are taken from studies of other relevant areas. For most *biological parameters* generic data are selected. These are often given a wide range to include the large variety, which occur between different areas. One exception to this is the yield values for which data relevant for the area are selected when available. Data about *living habits* are chosen to reflect Swedish conditions of today, which should also include those at the SFR-area. For the *radiological parameters*, dose conversion factors specified by the authorities are selected and the half-life of radionuclides is according to Firestone *et al*. /1999/.

In the following sections the data selected in the calculations are compiled. These data can also be found in Karlsson *et al.* /2001a/ and in Karlsson and Bergström /2001/ where motivations for the selection of values are treated in more detail.

8.4 Selected data

8.4.1 Geometrical data

The data selected for geometrical parameters are compiled in Table 8-1. These values are to a large extent site specific. An exception to this is the porosity of soil and peat for which general data are selected in lack of site specific information. For a detailed discussion about the selected parameter values see Karlsson *et al* /2001a/.

8.4.2 Physical/chemical data

This category of parameters describes physical and chemical states as well as processes that are of importance for the dispersion of radionuclides in the biosphere. The selected data for these parameters are compiled in Table 8-2 to Table 8-4.

The values selected for physical parameters are to a large extent site specific, see Table 8-2. An exception to this is the parameters for soil and peat for which generic values are selected.

Sorption/desorption of radionuclides to solid matter in different matrices (e.g. soil, peat or water and suspended matter) is modelled using element specific distribution coefficients (see Table 8-3 and Table 8-4). Such values can be found in the literature, but data for the same element often differ several orders of magnitude. This is not surprising since the measured values are depending on measuring techniques and detection limits. The sorption itself varies also with conditions such as water content, appearance of conquering matrices (often organic matter) and also with time. Because of this, wide ranges have been selected for all K_d-values (see Table 8-3and Table 8-4). These should very well include the conditions in soils in the area today as well as in the future.

Sorption/desorption is a time-dependent process and to consider this a specific parameter called Tk has been introduced. This parameter is the half-time to reach sorption equilibrium and has set to vary within a very wide range as it includes differences between elements as well as between matrices and also the large uncertainties in these estimated values. A log-triangular distribution is selected. Best estimate is set to a few hours (10^{-3} year), minimum set to a few minutes (10^{-5} year^{-1}) and maximum (10^{-1} year^{-1}) is based on the extremely slow cesium sorption to clay calculated from observed desorption rate and partitioning coefficient (e.g. Meili and Wörman /1996 and 1997/.

8.4.3 Biological data

The biological parameters used in the models to estimate exposure to humans are root uptake factors, translocation factors, bioaccumulation factors for aquatic biota and transfer coefficients for milk and meat. All these parameters are element specific and for all, except for translocation factors, a large range is often used. This is due to variability as well as uncertainty in the reported values. Root uptake, e.g., varies with soil type, weather conditions and of course with vegetation type. Here different values are specified for different kind of crops, see Table 8-5 and Table 8-6. The wide range should, anyhow, include variability in other conditions.

Generally, data about translocation of radionuclides deposited on vegetation surfaces to edible parts of crop is very limited. For many elements a best estimate of 10 %, varying from 1-30 % are selected as no information was found. This wide range should include the actual value. For elements which are known to be bioavailable (readily taken up in biota) some data has been found, see Table 8-7.

The validity of using transfer coefficients is discussed in IAEA /1994/ and in Ward and Johnson /1986/. Some of the difficulties include the need for equilibrium (with a few exceptions, most radionuclides will not have equilibrated in animal products before slaughter), metabolic homeostasis, effects of chemical and physical form of radionuclides and influence of animal age. In general, wide ranges are selected in this study to include these uncertainties as well as natural variability, see Table 8-8.

Values of bioaccumulation factors for a given element vary widely among organisms as well as environments. The documentation in literature of how these values are determined are often poor (Karlsson *et al.*, 2001b). One such uncertain factor is how the concentration of the element of interest in water has been obtained as it can be filtered or not before measuring the radioactivity. The part of the organism that has been analysed is also of importance, as elements tend to accumulate in different tissues. The chemical conditions of the water influence the uptake of radionuclides in freshwater biota. As can be seen in Table 8-9 wide ranges are selected for bioaccumulation factors to include this natural variability as well as the uncertainties and variations in reported values.

8.4.4 Living habits of humans and cattle

Values of parameters related to the production and consumption of food and water by cattle and humans are given in Table 8-10 and Table 8-11. Parameter values selected for calculating exposure from burning of peat are given in Table 8-12 and the time of exposure from contaminated ground is given in Table 8-11. As mentioned earlier data for these parameters are chosen to reflect Swedish conditions of today which should also include those at the SFR-area.

8.4.5 Radiological data

Radiological data are the only parameter category for which deterministic values are selected. The dose coefficients are surely connected with both variations and uncertainties, but in the literature no such information can be found. As it is beyond the knowledge of the authors to set up relevant ranges deterministic values are selected. The half-lives of radionuclides are known physical facts and are the parameters that are connected with least uncertainties of the parameters used in this study.

In Table 8-13 the half-lives and type of dominating decay is given for the radionuclides considered within the study. The dose coefficients for ingestion, inhalation and external exposure are also given in the table. These parameter values are not probabilistically

treated in the calculations. For sure there are uncertainties connected also to these kinds of data, but we have chosen not to give those as distributions since no information about uncertainties or variations is present.

8.4.6   Tables with selected data

Table 8-1. Selected geometrical data for modelling radionuclide transfer in the different biosphere systems from 2000 – 12000 AD

Parameter	Unit	Best estimate	Min – Max	Distr function	Reference/ Notation
Coast 1 and 3					
Model area (= part of Öregrundsgrepen)					
Area	km^2	11.2		Constant	Kautsky /2001/
Mean depth	m	9.5	8.5 – 10.5	T	Kautsky /2001/
Fraction acc. Bottom	-	0.22	0 – 0.44	T	Brydsten /1999b/
Öregrundsgrepen					
Area	km^2	456	433 – 479	T	Kautsky /2001/
Mean depth	m	11.2	10.2 – 12.2	T	Kautsky /2001/
Fraction accumulation bottom	-	0.3	0.15 – 0.6	T	Brydsten /1999b/
Baltic Sea					
Area	km^2	377400	370000 – 380000	T	SNA /1992/
Mean depth	m	56	52 – 60	T	SNA /1992/
Fraction acc. Bottom	-	0.3	0.15 – 0.5	T	Jonsson *et al.* /1990/
Model area, Öregrundsgrepen and Baltic Sea					
Depth of upper sediment	m	0.02	0.005 – 0.05	logT	Eckhell *et al.* /2000/
Coast 2					
Model area (= part of Öregrundsgrepen)					
Area	km^2	1.7	0.85 – 2.55	T	1,2
Mean depth	m	4.3	2.15 – 6.45	T	2,3
Fraction acc. Bottom	-	0.95	0.80 – 0.99	T	4
Öregrundsgrepen					
Area	km^2	228	114 – 342	T	2,5
Mean depth	m	7.5	3.75 – 11.25	T	2,5
Fraction acc. Bottom	-	0.9	0.75 – 0.95	T	4
Model area, Öregrundsgrepen and Baltic Sea					
Depth of upper sediment	m	0.02	0.005-0.05	logT	6
Lake					
Area	km^2	1.06	0.8 – 1.25	T	Brunberg and Blomqvist /2000/
Mean depth	m	1.7	1.4 – 2.1	T	Brunberg and Blomqvist /2000/
Fraction acc. Bottom	-	0.2	0 – 1.0	T	
Depth of upper sediment	m	0.02	0.005 – 0.05	logT	Eckhell *et al.* /2000/
Agricultural land					
Area	m^2	530 000	400 000 – 625 000	T	7
Depth of saturated zone	m	3	2 – 4	T	8
Saturated zone porosity	m^3/m^3	0.3	0.25 – 0.35	T	9
Depth of top soil	m	0.25	0.20 – 0.30	T	Haak /1983/
Top soil porosity	m^3/m^3	0.5	0.4 – 0.6	T	Wiklander /1976/
Deep soil porosity	m^3/m^3	0.5	0.4 – 0.6	T	Wiklander /1976/
Peat bog					
Peat area	m^2		0.24 – 1.25	U	10
Peat depth	m		0.7 – 2.1	U	11
Porosity of peat	m^3/m^3	0.9	0.8 – 0.95	T	Sharma and Forster /1993/

Notations to Table 8-1

1) Estimated from Brydsten /1999a/.

2) The range of this parameter is set +/- 50 % of the best estimate, a relatively wide interval, since the values are estimations from predictions of the future conditions and therefore associated with large uncertainty.

3) Between 2000 AD and 5000 AD when the lake is formed the mean depth of the water volume decreases from 9.5 to 1.7 m. If this decrease is assumed to be constant the mean depth at 4000 AD will be about 4.3 m

4) Brydsten L, pers. comm. 2000-12-11. The range is set by the authors

5) According to Brydsten /1999a/ the water area of Öregrundsgrepen is decreased to half of the area at 2000 AD and the volume will be decreased with two thirds. The mean depth is calculated according to this statement.

6) The same value as used for 2000 AD.

7) The area used for agricultural purposes is assumed to be available after drainage of the large lake which will arise within the area in the future /Kautsky, 2001/. It is assumed that half of the lake area is drained and cultivated. The lake area is set to 1.06 km^2 (best estimate range: 0.8 – 1.25 km^2), which gives an agricultural area of 530 000 m^2, ranging from 400 000 to 625 000 m^2.

8) The soil used for agricultural purposes is assumed to consist of the sediments deposited in accumulation zones when the area is a coastal area and later a lake /Kautsky, 2001/. The coastal and lake stages are assumed to remain for about 2 500 years each. The sedimentation in accumulation areas during the coastal period is about 1.8 kg dw/(m^2·year) and with a density of about 2 600 kg dw/m^3 and a porosity of about 50 % the sediment depth accumulated during these 2 500 year will be about 3.5 m. During the lake period another 0.5 m is added (sedimentation = 0.4 kg dw/(m^2·year). As the upper two layers (top soil and deep soil) together has a depth of 1 m the depth of the saturated zone is here set to 3 m, varying from 2 to 4m.

9) The porosity in aquifers may vary considerable between 30 to 60 % in loose deposits /Grip and Rodhe, 1985/. In order not to underestimate the upward transport of radionuclides 30 % is selected as a mean value, subjectively ranging from 25 to 40 %.

10) It is predicted that the large lake which will form in the area in the future /Kautsky, 2001/ will be gradually transformed into a mire. To estimate the extension of the mire is not easy. Here it is assumed that 30-100 % of the former lake basin will be transformed into a mire, hence the size of the mire is set to minimum 0.24 km^2 (30 % of the minimum lake area) and maximum 1.25 km^2 (100 % of maximum lake area). A uniform distribution is selected since it is not possible to make a better estimation.

11) Most Swedish peat bogs are about 2 meters deep (www.torvproducenterna.se/basfakta.html, 2000-08-04). The minimum depth to be classed as peat-bogs are 0.3 m. In this case the mire depth is set according to the depth of the lake basin which is predicted to be gradually transformed into a mire /Kautsky, 2001/. It is assumed that the depth of the mire will be at least half of the lake depth, i.e. 0.7 m (half of the minimum lake depth), and at most of the same depth, i.e. 2.1 m (maximum lake depth). A uniform distribution is selected since it is not possible to make a better estimation.

Table 8-2. Selected physical data for modelling radionuclide transfer in the different biosphere systems from 2000 – 12000 AD. The probability distribution selected is either Triangular or log Triangular.

Parameter	Unit	Best estimate	Min – Max	Distr. Function	Reference/Notation
Model area (= part of Öregrundsgrepen)					
Water retention time	year	$2.11 \cdot 10^{-3}$	$(1.05\text{-}4.22) \cdot 10^{-3}$	log T	Engqvist and Andrejev /1999/
Öregrundsgrepen					
Water retention time	year	0.033	0.030 – 0.036	T	Engqvist and Andrejev /1999/
Model area and Öregrundsgrepen					
Suspended matter	kg/m^3	$5 \cdot 10^{-3}$	$(2.5 - 10) \cdot 10^{-3}$	T	1
Sediment growth rate	m/year	0.01	0.004 – 0.02	log T	2
Baltic Sea					
Water retention time	year	22	15 – 30	T	SNA /1992/
Suspended matter	kg/m^3	$1 \cdot 10^{-3}$	$(0.5 - 2) \cdot 10^{-3}$	log T	1
Sediment growth rate	m/year	0.002	0.0008 – 0.005	log	2
Model area, Öregrundsgrepen and Baltic Sea					
Fine particle settling velocity	m/year	365	73 – 7300	log T	1
Lake					
Water retention time	year	0.24	0.17 – 0.31	T	Brunberg and Blomqvist /2000/
Suspended matter	kg/m^3	$2 \cdot 10^{-3}$	$(0.5 - 5) \cdot 10^{-3}$	log T	Lindström *et al.* /1999/
Sediment growth rate	m/year	0.004	0.001 – 0.010	log T	3
Fine particle settling velocity	m/year	183	36.5 – 3600	log T	4
Agricultural land					
Surface runoff	m^3/(m^2/year)	0.25	0.20 – 0.30	T	Lindborg and Schüldt /1998/
Water transport from groundwater to deep soil	m^3/(m^2/year)	0.2	0.1 – 0.3	log T	BIOMOVS /1996/
Water transport from deep soil to top soil	m^3/(m^2/year)	0.10	0.05 – 0.20	T	5
Water transport from deep soil to groundwater	m^3/(m^2/year)	0.2	0.1 – 0.3	T	6
Retention of irrigation water	m^3/m^2	0.003	0.001 – 0.005	T	Persson /1997/
Soil removal by erosion	kg/m^2/year	0.005	0.002 – 0.020	T	7
Soil density	kg/m^3	2650	2600 – 2700	T	Hillel /1980/
Bioturbation	kg/m^2/year	2	1 – 3	T	Müller-Leman and van Dorph /1996/
Weathering half-life	day	15	10 – 20	T	IAEA /1994/
Dust concentration in air	kg/m^3	$1 \cdot 10^{-4}$	$(0.3 - 3) \cdot 10^{-4}$	T	Haak /1983/
Peat bog					
Surface runoff	m^3/(m^2/year)	0.25	0.20 – 0.30	T	Lindborg and Schüldt /1998/
Density	kg d.w./m^3	100	80 – 120	T	Steinman and Shotyk /1997/
Relative dispersion factor	s/m^3	$1 \cdot 10^{-5}$	$(0.3 - 3) \cdot 10^{-5}$	log T	Widemo and Gyllander /1979/
Dust concentration in air	kg/m^3	$1 \cdot 10^{-4}$	$(0.3 - 3) \cdot 10^{-4}$	T	Haak /1983/
Well model					
Dilution volume (base case)	m^3	867	(496 – 1237)	T	8

Notations to Table 8-2

1) $Susp_B$ and V_{sink}: Gross sedimentation (= $Susp_B$ * V_{sink}) needs to balance observed sediment growth (see 2 below), which is about 1 or a few mm/y or approximately 0.1 kg m^{-2} y^{-1} in the open Baltic /SNA, 1992; Ilus *et al*. 1995; Eckhéll *et al*. 2000/, and about 1 cm/y in the SFR area, similar to other coastal archipelagos /Meili *et al*. 2000a and b; Ilus *et al*., 1995/. $Susp_B$ is supported by e.g. Pempkowiak *et al*. /1998/ and Nordvarg and Johansson /in prep/. V_{sink} is supported by suspended matter concentrations and sediment trap studies /Lindström *et al*., 1999; Weyhenmeyer *et al*., 1997; Meili unpubl./ and agrees with Stoke's law: V_{sink} = 0.2…20 m/d for silt 2…20 µm and <0.01…0.3 m/d for plankton 2…20 µm. For compatibility with coastal values, surface water values are given for the open Baltic (high $Susp_B$, low V_{sink}) rather than deep-water values (low $Susp_B$, high V_{sink}). The ranges are rough estimates of uncertainty in the annual mean over larger areas, while concentrations and fluxes can vary by over an order of magnitude within days, but also among sites /Weyhenmeyer *et al*., 1997/.

2) Values are based on the observed lamination structure and ^{137}Cs dating of over 100 coastal sediment cores in the region, e.g. Meili *et al*. /2000b/. The resulting apparent turnover time of the mixed upper sediment layer (around 2 cm, e.g. Eckhéll *et al*. /2000/) is about 2 years in coastal accumulation areas with a sediment growth rate of about 1 cm/year, and about 10 years in offshore areas with a growth rate of 0.2 cm/year.

3) As in the coastal model this value is estimated from sediment mass balance calculations of the lake. A growth rate of 0.4 cm/year corresponds to a turnover time for the upper sediment layer (2 cm) of about 5 years

4) The particle settling velocity is i.a. depending on the size and density of the settling particles. In lakes a large fraction of the particles and sediments is organic matter which tends to sink at a slower rate than mineral particles of the same size. A mean value half as large as that used in the coastal model is therefore selected and the range is adopted from the same parameter in the coastal model.

5) Transport of 100 mm from deep soil to the top layer, compared to 200 mm from groundwater to deep soil, is selected, as e.g. the influence of capillary rise will decrease when the distance to the groundwater table increases. The upper soil layer also receives water through precipitation. The upward transport of water in soil is also driven by the water uptake of vegetation. Part of the water is taken up directly by the plants, but a fraction will also remain within the upper soil layer (which is the fraction modelled).

6) Equilibrium is assumed to have been established so the upward flow of water from the groundwater zone to the deep soil is assumed to be of the same size as the flow in opposite direction. This assumption is reasonable since the soil is assumed to be drained so the level of the groundwater surface is rather constant.

7) The importance of erosion for transport of soil varies considerable. An investigation of erosion in southern Sweden presents losses of 0.5 to 300 tons per ha /Alström and Bergman, 1986/. A later investigation showed much lower values, from 0.001 to 80 tons per ha /Alström *et al*, 1991/. Erosion has also been studied as transport of suspended matter in running waters /Nilsson, 1972/. The results indicate annual losses from 10 up to hundreds of kg per ha. When the parameter range was estimated the extreme values were excluded.

8) This volume is assumed to be the same as the annual amount of water taken from the well. The critical group for which the dose is calculated consists of 5-10 people, living on a small farm. It is assumed that these people drink 1.6 liters of water per day (600 liters/year). In addition to this each person consumes 200 liters/day for washing, showering etc. The total water consumption for the group becomes 1-2 m^3/day. It is also assumed that the farm has 5-10 cows and that each cow consumes 65-75 liters/day, which gives a total of 325–750 liters/day. Furthermore, the water from the well is used for irrigation of a garden plot. It is assumed that the garden plot is irrigated 6-14 times per year. The volume of water used at each time is between 0.014-0.067 m^3 of water per m^2 of garden. The area of the garden is assumed to be between 150 – 250 m^2. Hence, the total volume used for irrigation will be between 12.6 m^3/year and 234.5 m^3/year. Thus, the total use of water by the small farm is between 1.36-3.39 m^3/day (496–1 237 m^3/year). The arithmetic average value of these two numbers is 2.375 m^3/day (867 m^3/year).

Table 8-3. Selected distribution coefficients (K_d-values) for soil and peat (m^3/kg dry weight). The probability function for all values is log Triangular.

Element	Soil; K_d (m^3/kg d.w.)			Peat; K_d (m^3/kg d.w.)		
	Best estimate	Min – Max	Reference	Best estimate	Min – Max	Reference
H	-	-	1)	-	-	1)
C	0.001	0.0004 – 0.01	2)	0.07	0.007 – 0.7	11)
Cl	0.001	0.0001 – 0.01	3)	0.01	0.001 – 0.1	12)
Co	1	0.01 – 20	4)	1	0.05 – 2	4)
Ni	0.5	0.05 – 5	4)	1	0.2 – 7	4)
Se	0.01	0.001 – 0.1	5)	2	0.2 – 20	4)
Sr	0.01	0.001 – 0.1	4)	0.2	0.004 – 6	4)
Zr	1	0.1 – 10	4)	7	0.7 – 70	4)
Nb	0.5	0.005 – 5	4)	2	0.2 – 20	4)
Mo	0.1	0.01 – 1	4)	0.03	0.003 – 0.3	4)
Tc	0.005	0.001 – 0.01	6)	0.002	0.00004 – 0.06	4)
Pd	0.2	0.02 – 2	4)	0.7	0.07 – 7	4)
Ag	0.1	0.01 – 1	4)	20	2 – 90	4)
Cd	0.1	0.002-3	4)	0.8	0.008-80	4)
Sn	0.1	0.05 – 0.5	7)	2	0.2 – 20	4)
I	0.3	0.1 – 1.0	8)	0.03	0.003 – 0.3	4)
Cs	1	0.1 – 10	9)	0.3	0.1 – 3	4)
Sm	1	0.1 – 10	4)	3	0.3 – 30	4)
Eu	10	1 – 100	9)	1	0.05-20	13)
Ho	1	0.1 – 10	4)	3	0.3 – 30	4)
U	0.1	0.01 – 1	10)	0.4	0.003 – 4	4)
Pu	5	0.1 – 10	9)	2	0.2 – 20	4)
Am	2	0.2 – 20	4)	100	10 – 1000	4)
Cm	10	1 – 100	4)	10	1 – 100	4)

1) Hydrogen does not sorb to particle matter and therefore no effort has been put on finding K_d-values since they are missing in e.g. IAEA /1994/.
2) Andersson *et al* /1982/
3) McKinley and Scholtis /1992/
4) IAEA /1994/
5) Extracted from Coughtrey *et al.* /1985/
6) Estimated from Hoffman and Baes /1979/
7) Tin is assumed to be analogous with Pb for which data orginally was taken from Jiskra /1985/. This study refers to Wuschke *et al.* /1981/
8) The best estimate is calculated from a transfer rate used in Bergström and Wilkens /1983/.The transfer rate was extracted from Kantelo *et al.* /1981/.
9) Coughtrey *et al.* /1985/
10) In Grogan /1985a/ this value was used with reference to Parker and Grant /1979/ and Dahlman *et al* /1976/.
11) Davis *et al.* /1993/
12) No value was found in IAEA /1994/ so an estimation was performed. Assuming that chlorine behaves like the elements in the same column in the periodic table a K_d-value close to that used for iodine has been used.
13) Data is lacking for this uncommon element and as Eu-152, Eu-154 and Eu-155 have short half-live it has not been of interest in any of the safety assessments performed by the authors and therefore no effort has been placed on finding data. NCRP /1996/ implies a behaviour similar to Co and Nb in aquatic environment and here it is assumed that this is the case also in organic soil. Because of the short half-live they are important for dose to humans in a short time perspective and to use a conservative approach the lowest K_d-value of these two (that of Co) is selected so that a larger amount should be available for exposure to humans during the coastal stage

Table 8-4. Selected distribution coefficients (K_d-values) for suspended matter in lakes and in brackish water (m^3/kg dry weight). The probability function for all values is log Triangular

Element	Suspended matter, lake; K_d (m^3/kg d.w.)			Suspended matter, Baltic sea; K_d (m^3/kg d.w.)		
	Best estimate	Min – Max	Reference	Best estimate	Min – Max	Reference
H	-	-	1)	0.001	0.00005 – 0.01	9)
C	0.001	0.0001 – 0.01	2)	0.001	0.0001 – 0.01	3)
Cl	1	0.1 – 10	3)	0.001	0.0001 – 0.01	9)
Co	5	1 – 70	4)	100	1 – 200	10)
Ni	10	1 – 100	3)	10	1 – 100	3)
Se	5	1 – 10	5)	5	1 – 10	5)
Sr	1	0.1 – 10	4)	0.1	0.01 – 1	11)
Zr	1	0.1 – 10	4)	50	5 – 500	5)
Nb	10	1 – 100	3)	10	1 – 100	5)
Mo	0.001	0.0001 – 0.01	6)	0.001	0.0001 – 0.01	6)
Tc	0.1	0.01 – 1	5)	0.1	0.01 – 1	5)
Pd	2	0.2 – 20	3)	10	1 – 100	3)
Ag	2	0.2 – 20	3)	1	0.1 – 10	12)
Cd	0.1	0.01-1	7)	5	1-100	9)
Sn	50	10 – 100	2)	50	10 – 100	2)
I	0.3	0.1 – 1	5)	0.3	0.1 – 1	5)
Cs	10	1 – 100	5)	10	1 – 100	5)
Sm	5	0.5 – 50	3)	100	10- 1000	3)
Eu	0.5	0.05-5	4)	10	1 – 100	13)
Ho	0.3	0.03 – 3	3)	0.1	0.01 – 1	3)
U	10	1 – 100	8)	10	1 – 100	8)
Pu	100	10 – 1000	5)	100	10 – 1000	5)
Am	5	0.5 – 50	4)	10	1 – 100	5)
Cm	5	0.1 – 70	4)	1000	10 – 2000	14)

1) Hydrogen does not sorb to particle matter to a large extent and therefore no effort has been put on finding K_d-values since they are missing in e.g. IAEA /1994/.

2) Bergström and Nordlinder /1990b/

3) McKinley and Scholtis /1992/

4) IAEA /1994/

5) Coughtrey *et al*. /1985/

6) The best estimate is taken from Aggeryd and Bergström /1990/. In that report the same K_d-values were used for sediments as for soil. The value are orginally from Jiskra /1985/ which refers to Inoue and Morisawa /1974/. The same value is selected for freswater and brackish water.

7) NCRP /1996/

8) A distribution coefficient in lakes in northern Sweden of 43 m^3/kg (mean value) was reported by Holm /1981/ and a range of 0.2-250 m^3/kg was given by Agnedal /1982/ according to Bergström and Wilkens /1983/. A value of 10 m^3/kg has been extracted. The values for fresh waters is selected for the Baltic sea as well.

9) IAEA /1985/

10) Bergström and Nordlinder /1993/

11) The best estimate is derived from Bergström and Nordlinder /1990a/ which treats lake water. It is most possible that this study has used the K_d-value for fresh water used in Bergström and Puigdomenech /1987/ (0.1 m^3/kg). This value is orginally extracted from Kenna /1980/.

12) The best estimate and range are defined in Bergström and Nordlinder /1993/. The K_d-values in that study were extracted from Coughtrey *et al* /1985/, Puigdomenech and Bergström /1995/ and McKinley and Scholtis /1991/.

13) Data is lacking for this uncommon element, but NCRP /1996/ implies a behaviour similar to Co and Nb in aquatic environment. Since Eu has a short half-life it is only important for dose to humans in a short time perspective and to use a conservative approach the lowest K_d-value of these two (that of Nb) is selected so that a larger amount should be available for exposure to humans during the coastal stage.

14) Best estimate and range defined in Bergström and Nordlinder /1993/. The K_d-values in that study were extracted from Coughtrey *et al* /1985/, Puigdomenech and Bergström /1995/ and McKinley and Scholtis /1991/.

Table 8-5. Selected root uptake factors for pasturage (grass and fodder)) and for cereals. The probability function selected for all values is log Triangular except for Cl where it is Triangular

Element	Pasturage (kg d.w.soil/kg d.w.fodder)			Cereals (kg d.w.soil/kg w.w.cereal)		
	Best estimate	Min – Max	Reference	Best estimate	Min – Max	Reference
H	50	20 – 80	1)	50	20 – 80	1)
C	No root uptake considered			No root uptake considered		
Cl	30	10 – 100	2)	30	9 – 90	2)
Co	0.1	0.01 – 1	3)	0.1	0.01 – 1	3)
Ni	0.2	0.02 – 2	4)	0.03	0.003 – 0.3	4)
Se	20	1 – 30	2)	20	0.9 – 30	2)
Sr	1	0.4 – 3	4)	0.2	0.02 – 1	4)
Zr	0.001	0.0001 – 0.01	4)	0.0009	$9 \cdot 10^{-5}$ – 0.009	4)
Nb	0.005	0.0005 – 0.05	5)	0.004	0.0004 – 0.04	5)
Mo	0.8	0.08 – 8	4)	0.7	0.07 – 7	4)
Tc	8	0.8 – 80	4)	0.6	0.06 – 3	4)
Pd	0.2	0.02 – 2	6)	0.03	0.003 – 0.3	6)
Ag	0.5	0.05 – 4	7)	0.4	0.04 – 3	7)
Cd	5	0.5-50	8)	5	0.5-50	8)
Sn	0.1	0.01 – 2	9)	0.4	0.01 – 1	9)
I	0.6	0.06 – 6	10)	0.1	0.01 – 1	13)
Cs	0.2	0.02 – 2	4)	0.02	0.002 – 0.2	4)
Sm	0.01	0.001 – 0.1	11)	0.0001	$1 \cdot 10^{-5}$ – 0.001	11)
Eu	0.01	0.001 – 0.1	11)	0.0002	$2 \cdot 10^{-5}$ – 0.002	11)
Ho	0.001	0.0001 – 0.01	12)	0.0001	$1 \cdot 10^{-5}$ – 0.001	12)
U	0.02	0.002 – 0.2	4)	0.001	0.0001 – 0.01	4)
Pu	0.0004	$5 \cdot 10^{-5}$ – 0.7	4)	$7 \cdot 10^{-6}$	$7 \cdot 10^{-7}$ – $7 \cdot 10^{-5}$	4)
Am	0.001	0.0005 – 0.2	4)	$2 \cdot 10^{-5}$	$2 \cdot 10^{-6}$ – 0.0002	4)
Cm	0.001	0.0001 – 0.004	4)	$2 \cdot 10^{-5}$	$1 \cdot 10^{-6}$ – 0.0003	4)

1) Calculated considering the same concentration of tritium in soil water as in water in plant.
2) Coughtrey *et al*. /1985/
3) The number studies concerning cobalt is limited. Data given in IAEA /1994/ and in Ng *et al* /1982/ is of the same magnitude. The data selected are extracted from these publications.
4) IAEA /1994/
5) Davis *et al*. /1993/
6) Due to lack of data the same values as for nickel are selected, as recommended in Bergström *et al* /1986/ referring to Grogan /1985b/. Pt is considered to be a better analogue for Pd /Moody, 1982/, but no data were available for this element either.
7) The best estimates and ranges are defined in Bergström *et al* /1991/. Silver is found in about the same concentrations in vegetation as in soil /Coughtrey et al, 1985; Bowen, 1979/. Very high concentrations have been found in flour though. In Coughtrey *et al* /1985 is a general value of 1.0 kg/kg recommended which is said to be a conservative value. This value is also recommended by IAEA /1982/. Considering this it is recommended in Bergström *et al* /1991/ to use a value of 0.5 kg/kg as best estimate for pasturage. For other crops this value is converted to wet weight. As a value of 1 is said to be conservative a maximum value four times that value is selected. The minimum value selected is ten times lower than the best estimate.
8) NCRP /1996/
9) The root uptake factors for tin were updated in Bergström *et al* /1986/ as justified by data in Coughtrey *et al* /1983/. Here a value about 1 is recommended, but a lower value is selected.
10) Deitermann *et al* /1989/
11) The best estimates are according to Baker *et al* /1976/, Miller *et al* /1980/ and Coughtrey and Thorne /1983a/. The minimum and maximum values of the ranges are ten times lower and higher, respectively, of the best estimate.
12) The best estimates are according to Baker *et al* /1976/ and Coughtrey and Thorne /1983a/. The value for pasturage was given for lanthanides in general. The minimum and maximum values of the ranges are ten times lower and higher, respectively, of the best estimate
13) Robens *et al* /1988/

Table 8-6. Selected root uptake factors for root crops and for vegetables. The probability function selected for all values is log Triangular except for H and Cl where it is Triangular

Element	Root crops (kg d.w.soil/kg w.w.crops)			Vegetables (kg d.w.soil/kg w.w.vegetab)		
	Best estimate	Min – Max	Reference	Best estimate	Min – Max	Reference
H	10	5 – 20	1)	10	5 – 20	1)
C	No root uptake considered			No root uptake considered		
Cl	6	2 – 20	2)	3	1 – 10	2)
Co	0.01	0.001 – 0.1	3)	0.01	0.001 – 0.1	3)
Ni	0.04	0.004 – 0.4	4)	0.02	0.002 – 0.2	4)
Se	4	0.2 – 6	2)	2	0.1 – 3	2)
Sr	0.06	0.01 – 0.3	4)	0.3	0.003 – 3	4)
Zr	0.0002	$2 \cdot 10^{-5}$ – 0.002	4)	0.0001	$1 \cdot 10^{-5}$ – 0.001	4)
Nb	0.001	0.0001 – 0.01	5)	0.0005	$5 \cdot 10^{-5}$ – 0.005	5)
Mo	0.2	0.02 – 2	4)	0.08	0.008 – 0.8	4)
Tc	0.05	0.005 – 0.5	4)	20	0.1 – 80	4)
Pd	0.04	0.004 – 0.4	6)	0.02	0.002 – 0.2	6)
Ag	0.2	0.02 – 1	3)	0.1	0.01 – 0.8	3)
Cd	1	0.1-10	7)	0.5	0.05-5	7)
Sn	0.06	0.01 – 1	8)	0.05	0.01 – 1	8)
I	0.01	0.001 – 1	9)	0.03	0.003 – 0.3	9)
Cs	0.02	0.002 – 0.2	4)	0.02	0.002 – 0.2	4)
Sm	$4 \cdot 10^{-5}$	$4 \cdot 10^{-6}$ – 0.0004	10)	0.003	0.0003 – 0.03	10)
Eu	$6 \cdot 10^{-5}$	$6 \cdot 10^{-6}$ – 0.0006	10)	0.003	0.0003 – 0.03	10)
Ho	$9 \cdot 10^{-5}$	$9 \cdot 10^{-6}$ – 0.0009	11)	0.003	0.0003 – 0.03	11)
U	0.003	0.0003 – 0.03	4)	0.001	0.0001 – 0.01	4)
Pu	$3 \cdot 10^{-5}$	$3 \cdot 10^{-6}$ – 0.0003	4)	$2 \cdot 10^{-5}$	$2 \cdot 10^{-6}$ –0.0002	4)
Am	$4 \cdot 10^{-5}$	$4 \cdot 10^{-6}$ – 0.0004	4)	$7 \cdot 10^{-5}$	$7 \cdot 10^{-6}$ – 0.0007	4)
Cm	$3 \cdot 10^{-5}$	$2 \cdot 10^{-6}$ – 0.0005	4)	0.0002	$2 \cdot 10^{-5}$ – 0.002	4)

1) Calculated considering the same concentration of tritium in soil water as in water in plant.
2) Coughtrey *et al.* /1985/.
3) The number studies concerning cobalt is limited. Data given in IAEA /1994/ and in Ng *et al* /1982/ is of the same magnitude. The data selected is extracted from these publications.
4) IAEA /1994/
5) Davis *et al.* /1993/
6) Due to lack of data the same values as for nickel are selected, as recommended in Bergström *et al* /1986/ referring to Grogan /1985b/. Pt is considered to be a better analogue for Pd /Moody, 1982/, but no data were available for this element either.
7) NCRP /1996/
8) The root uptake factors for tin were updated in Bergström *et al* /1986/ as justified by data in Coughtrey *et al* /1983/. In that study a value about 1 is recommended, but a lower value is selected.
9) Robens *et al* /1988/
10) The best estimates are according to Baker *et al* /1976/, Miller *et al* /1980/ and Coughtrey and Thorne /1983a/. The minimum and maximum values of the ranges are ten times lower and higher, respectively, of the best estimate.
11) The best estimates are according to Baker *et al* /1976/ and Coughtrey and Thorne /1983a/. The value for pasturage was given for lanthanides in general. The minimum and maximum values of the ranges are ten times lower and higher, respectively, of the best estimate

Table 8-7. Selected translocation factors from surface to edible parts of cereals and root crops. The probability function selected for all values is log Triangular.

Element	Translocation factor (m^2/kg w.w.)		
	Best estimate	Min – Max	Reference
H	0.1	0.01 – 0.3	1)
C	0.1	0.01 – 0.3	1)
Cl	0.1	0.01 – 0.3	1)
Co	0.2	0.1 – 0.3	2)
Ni	0.01	0.005 – 0.04	3)
Se	0.1	0.01 – 0.3	2)
Sr	0.4	0.1 – 0.7	2)
Zr	0.1	0.01 – 0.3	1)
Nb	0.2	0.1 – 0.3	2)
Mo	0.1	0.01 – 0.3	2)
Tc	0.5	0.4 – 0.6	2)
Pd	0.1	0.01 – 0.3	1)
Ag	0.1	0.01 – 0.3	1)
Cd	0.02	6E-05-0.05	4)
Sn	0.1	0.01 – 0.3	1)
I	0.1	0.05 – 0.2	5)
Cs	0.2	0.1 – 0.3	4)
Sm	0.1	0.01 – 0.3	1)
Eu	0.02	0.01 – 0.03	6)
Ho	0.1	0.01 – 0.3	1)
U	0.1	0.01 – 0.3	1)
Pu	0.02	0.01 – 0.03	2)
Am	0.01	0.005 – 0.02	2)
Cm	0.02	0.01 – 0.03	7)

1) Since data is lacking a best estimate of 10 % is selected as for many other elements for which other data has not been found. A rather wide range is selected, as the uncertainty is high.
2) Coughtrey *et al* /1985/
3) Data is scarce, but according to Coughtrey *et al* /1985/ it is assumed that very little nickel is transferred to edible parts. Therefore a low value is selected.
4) IAEA /1994/
5) Coughtrey *et al* /1983/
6) Bergström and Nordlinder /1991/
7) In lack of data the same values as for plutonium is selected.

Table 8-8. Selected transfer coefficients for uptake in cow milk and meat from daily intake. The probability function selected for all values is log Triangular except for transfer of Cl to milk where it is Triangular

Element	Milk (day/l)			Meat (day/kg)		
	Best estimate	Min – Max	Reference	Best estimate	Min – Max	Reference
H	0.02	0.01 – 0.03	1)	0.01	0.001 – 0.1	11)
C	0.01	0.005 – 0.02	2)	0.03	0.015 – 0.060	2)
Cl	0.017	0.015 – 0.02	3)	0.02	0.01 – 0.04	3)
Co	0.0003	$6 \cdot 10^{-5}$ – 0.01	3)	0.01	$4 \cdot 10^{-5}$ – 0.07	3)
Ni	0.02	0.002 – 0.05	3)	0.005	0.0005 – 0.05	3)
Se	0.004	0.0004 – 0.04	4)	0.015	0.0001 – 0.02	4)
Sr	0.0028	0.001 – 0.003	3)	0.008	0.0003 – 0.01	3)
Zr	$6 \cdot 10^{-7}$	$6 \cdot 10^{-8}$ – $6 \cdot 10^{-6}$	3)	$1 \cdot 10^{-6}$	$1 \cdot 10^{-7}$ – 0.01	3)
Nb	$4 \cdot 10^{-7}$	$1 \cdot 10^{-7}$ – $4 \cdot 10^{-6}$	3)	$3 \cdot 10^{-7}$	$3 \cdot 10^{-8}$ – 0.01	3)
Mo	0.002	0.0002 – 0.02	3)	0.001	0.0001 – 0.01	3)
Tc	$2 \cdot 10^{-5}$	$1 \cdot 10^{-5}$ – 0.001	3)	0.0001	$1 \cdot 10^{-5}$ – 0.001	3)
Pd	0.001	0.0001 – 0.01	5)	0.001	0.0001 – 0.01	5)
Ag	$5 \cdot 10^{-5}$	$5 \cdot 10^{-6}$ – 0.0005	3)	0.003	0.002 – 0.006	3)
Cd	0.0001	$1 \cdot 10^{-5}$ – 0.001	6)	0.0004	$4 \cdot 10^{-5}$ – 0.004	3)
Sn	0.001	0.0001 – 0.01	7)	0.01	0.001 – 0.1	7)
I	0.01	0.001 – 0.04	3)	0.04	0.007 – 0.05	3)
Cs	0.008	0.001 – 0.03	3)	0.05	0.01 – 0.06	3)
Sm	$2 \cdot 10^{-5}$	$2 \cdot 10^{-6}$ – 0.0002	8)	0.005	0.0005 – 0.05	9)
Eu	$2 \cdot 10^{-5}$	$2 \cdot 10^{-6}$ – 0.0002	8)	0.006	0.0006 – 0.06	8)
Ho	$2.5 \cdot 10^{-6}$	$3.0 \cdot 10^{-7}$ – $3.0 \cdot 10^{-5}$	9)	0.005	0.0005 – 0.05	9)
U	0.0004	$7 \cdot 10^{-5}$ – 0.0006	3)	0.0003	$3 \cdot 10^{-5}$ – 0.003	3)
Pu	$1 \cdot 10^{-6}$	$3 \cdot 10^{-9}$ – $3 \cdot 10^{-6}$	3)	$1 \cdot 10^{-5}$	$2 \cdot 10^{-7}$ – 0.0002	3)
Am	$2 \cdot 10^{-6}$	$4 \cdot 10^{-7}$ – $2 \cdot 10^{-5}$	3)	$4 \cdot 10^{-5}$	$4 \cdot 10^{-6}$ – 0.0001	3)
Cm	$2 \cdot 10^{-5}$	$2 \cdot 10^{-6}$ – 0.0002	10)	$2 \cdot 10^{-5}$	$2 \cdot 10^{-6}$ – 0.0002	10)

1) Van den Hoek *et al* /1979/ has studied the metabolism of tritium in cattle. The studies showed that secretion of H-3 to milk was 0.016 (average value). This value is rounded off and a narrow range is selected since tritium is a constituent of water and therefore the variation is considered not to be so large

2) The best estimates are taken from Bergström and Puigdomenech /1987/ with reference to unpublished results by Bergström and Hoffman. The results has not been published, but the value selected is in accordance with that used by Davis *et al* /1993/; $1.5 \cdot 10^{-2}$ day/L for milk and $6.4 \cdot 10^{-2}$ day/kg for meat. Values for carbon are based on the amounts of the stable element in different medium and organisms and as that content do not vary very much for cattle and grass respectively a rather narrow range is selected.
The range used for meat in SR 97 ($1 \cdot 10^{-3}$ day/L – $1 \cdot 10^{-1}$ day/L) is decreased in accordance to this.

3) IAEA /1994/

4) Davis *et al.* /1993/

5) The amount of data concerning the metabolism of palladium is not large, e.g. no values are found in IAEA /1994/. The values given in NCRP /1996/ and those used in Davis *et al* /1993/ differ very much. For milk a value of $1 \cdot 10^{-4}$ day/L is presented by NCRP and $1 \cdot 10^{-2}$ day/L is used by Davis *et al.* The values for meat are $2 \cdot 10^{-4}$ day/kg /NCRP/ and $4 \cdot 10^{-3}$ day/kg /Davis *et al.*/. The ranges selected here are set to include these values.

6) An equilibrium forage-to-milk transfer coefficient of $1 \cdot 10^{-4}$ day/l is suggested in Coughtrey *et al.* /1985/. It is also stated that this value is larger than suggested by available experimental results and may require modification. To use a conservative approach this value is selected.

7) NCRP /1996/

8) Miller *et al* /1980/

9) Baker *et al* /1976/

10) IAEA /1982/

11) In Bergström *et al* /1991/ a special model for calculation of dose from tritium was set up. The transfer coefficients used were taken from Neil /1991/. A transfer coefficient from vegetation to meat of 0.2 kg/kg grass was used. In SR 97 and SAFE another model approach is used. Instead of this kind of transfer coefficient, a transfer coefficient to meat related to the cow's consumption of cereals and grass is used (not the whole amount of vegetation present in the area as in the former study). With a consumption rate of about 20 kg/day (5 kg grass and 12 kg cereals per day in SR 97 and 8.5 kg grass and 11 kg cereals per day in SAFE) and a transfer coefficient of 0.01 day/kg this match the transfer coefficient from vegetation to meat given by Neil /1991/. The range used in SR 97 ($1 \cdot 10^{-3}$ – $1 \cdot 10^{-1}$) is decreased in SAFE. In accordance to what is said about the transfer coefficient to milk a narrow range is selected since tritium is a constituent of water and therefore the variation is considered not to be so large.

Table 8-9. Selected bioaccumulation factors for fish in fresh water and in brackish water. The probability function selected for all values is log Triangular except for H and Cl in brackish water where it is Triangular.

Element	Fresh water (l/kg fish)			Brackish water (l/kg fish)		
	Best estimate	Min – Max	Reference	Best estimate	Min – Max	Reference
H	1	0.5 – 2	1)	1	0.5 – 2	9)
C	50 000	5000 – 50 000	2)	2000	2000 – 3000	10)
Cl	50	10 – 100	3)	1	0.1 – 10	3)
Co	300	10 – 400	1)	300	30 – 500	11)
Ni	100	10 – 1000	1)	300	30 – 500	12)
Se	2000	500 – 5000	4)	4000	2000 – 8000	3)
Sr	60	10 – 1000	1)	30	10 – 100	13)
Zr	200	3 – 300	1)	100	10 – 200	14)
Nb	300	100 – 30 000	1)	100	10 – 500	15)
Mo	10	1 – 100	1)	10	1 – 50	16)
Tc	20	2 – 80	1)	30	1 – 100	17)
Pd	100	10 – 1000	5)	10	1 – 100	18)
Ag	5	0.2 – 10	1)	500	100 – 1000	19)
Cd	20	2-200	3)	200	20-2000	3)
Sn	3000	300 – 30 000	1)	1000	100 – 10 000	3)
I	200	10 – 500	6)	30	10 – 100	20)
Cs	10 000	5000 – 20 000	7)	200	100 – 500	21)
Sm	25	2 – 300	8)	30	3 – 300	8)
Eu	50	10-200	1	100	10 – 1000	18)
Ho	25	2.5 – 300	8)	25	2.5 – 300	8)
U	10	2 – 50	1)	50	10 – 100	22)
Pu	30	4 – 300	1)	30	5 – 50	23)
Am	30	10 – 300	1)	100	10 – 200	24)
Cm	30	10 – 300	1)	50	10 – 300	25)

1) IAEA /1994/

2) Bergström and Nordlinder /1990b/

3) Coughtrey *et al*. /1983/

4) Extracted from Coughtrey *et al* /1983/

5) Due to lack of data the same values as for nickel is selected, as recommended in Bergström *et al* /1986/ referring to Grogan /1985b/. That study concerns root uptake, but a similar behaviour between palladium and nickel can also be expected in aquatic environments. Pt is considered to be a better analogue for Pd /Moody, 1982/, but no data were available for this element either

6) Poston and Klopfer /1986/

7) Value valid for oligotrophic freshwater. In Bergström and Nordlinder /1990b/ a value of 5 000 L/kg is used based on a number of studies. Kohlemainen /1968/ gives bioaccumulation factors in the range of 200-2 000 L/kg for piscivorous fish in eutrophic (nutrient rich) lake systems and Neumann /1985/ gives a generic value of 200 L/kg. Vanderploeg *et al* /1975/ gives the transfer at steady state as a function of the potassium concentration in water; 15 000/[K] for piscivorous fish. Studies of the Chernobyl fallout in the same type of lakes give a value of about 5 000 L/kg for species used as food /Bergström and Nordlinder, 1989/. In Bergström *et al* /1999/ a best estimate of 10 000 L/kg was used for oligotrophic lakes (with low potassium content). The value is higher than for eutrophic lakes in accordance to the function set up by Vanderploeg /1975/.

8) USNRC /1977/

9) A best estimate of 1 L/kg was recommended in Bergström and Nordlinder /1992/ based on Strand *et al* /1976/ and Blaylock and Frank /1979/.

10) Based on the carbon content in fresh fish and the concentrations in surrounding water a bioaccumulation factor of about 2 400 L/kg is gained for the Baltic Sea (calculated from carbon amounts in Hesböl *et al* 1990/. The factor gets about 1 800 L/kg for the Swedish West coast. A best estimate of 2 000 L/kg is therefore selected.

11) In Bergström and Nordlinder /1992/ a best estimate of 300 L/kg and a range of 20-400 L/kg is recommended for brackish water. In Coughtrey and Thorne /1983b/ a value of 3 L/kg is recommended for fish flesh, whereas Poston and Klopfer /1986/ recommends much higher values (100 L/kg for marine environments and 330 L/kg for freshwater fish when water quality is unknown).

12) The values are recommended in Bergström and Nordlinder /1992/. The accumulation of nickel in muscles of marine animals is limited (Coughtrey and Thorne /1983b/). Due to the small amount of data these authors recommend data for cobalt to be used instead. The low uptake has also been confirmed by Tjaelve *et al* /1988/.

13) The value is taken from Bergström and Nordlinder /1992/. This study recommends a best estimate of 30 L/kg for brackish waters based on recommendations in Patzer /1976/ of bioaccumulation factors of 3-10 L/kg for fresh water fish and 0.9-90 L/kg for marine fish. The range given here is set so wide that it includes these two ranges.

14) The best estimate and range are taken from Bergström and Nordlinder /1992/ which refers to Coughtrey and Thorne /1983a/. Here a bioaccumulation factor of 200 L/kg for whole fish and muscle for long-time exposure is recommended whereas a factor of 10 is recommended for muscle concerning short-time exposure

15) The best estimate and range are taken from Bergström and Nordlinder /1992/. The bioaccumulation factor presented in Thompson *et al* /1972/ is 30 000 L/kg which is considerably higher than what has been found by others /ScottRussel, 1966 and Ancellin *et al*, 1979/. The latter has measured factors between 1 and 30 in in-situ studies and between 110 and 260 in experiments. Freke /1967/ used a factor of 100 in his calculations

16) The best estimate and range are taken from Bergström and Nordlinder /1992/ which refers to Short *et al* /1971/.

17) The best estimate and range are taken from Bergström and Nordlinder /1992/. Blaylock and Frank /1982/ measured bioaccumulation factors from 11 to 121 for different fish species in a small pond. Laboratory experiments with marine fish show lower factors, about 2 L/kg /Masson *et al*, 1989/. Pentreath measured an average value of 11 L/kg /Pentreath, 1981/ whereas Verthé *et al* /1986/ measured a bioaccumulation factor of 0.2 in marine environment for Serranus cabrilla. As is said in Beasley and Lorz /1986/ the uptake of technetium is considered to be low in fish.

18) NCRP /1996/

19) The best estimate and range are taken from Bergström and Nordlinder /1992/ which refers to Coughtrey and Thorne /1983b/. The value recommended for brackish environments in Bergström and Nordlinder /1992/ is that for freshwater anyway.

20) The best estimate and range are taken from Bergström and Nordlinder /1992/. A best estimate of 30 is given for freshwater fish in Coughtrey *et al* /1983/.

21) The best estimate and range are taken from Bergström and Nordlinder /1992/. This study refers to Evans /1985 and 1991/ and Grimås /1991/ for a bioaccumulation factor of about 200 L/kg for fish from the Baltic Sea

22) The best estimate and range are defined in Bergström and Nordlinder /1990b/. The best estimate is the value recommended for freshwater fish muscle in Poston and Klopfer /1986/. In Hoffman /1988/ factors mostly under one are obtained, but the higher value was chosen in order to be conservative.

23) The range and best estimate are defined in Bergström and Nordlinder /1992/. Bioaccumulation factors between 0.9 and 550 L/kg have been recorded from the Marhall Islands /Noshkin *et al*, 1981/ whereas factors for freshwater fish has been reported from i.a. Vanderborght /1985/. Also here the variation was large; from 0.04 L/kg up to above 200. According to Eyman and Trabalka /1980/ the uptake decreases with increasing position in the food web. They recommend a factor of 250 for bottom dwelling fishes, a factor of 25 for plankton feeding species and a factor of 5 for piscivorous species. As it is mainly piscivorous species that are consumed by humans a best estimate of 30 is selected.

24) The range and best estimate are defined in Bergström and Nordlinder /1992/. The available amount of data concerning bioaccumulation of americium is scarce. Poston and Klopfer /1986/ recommends a value of 100 L/kg for freshwater fish. In the same reference values of bioaccumulation factors depending on the trophic level of the fish is also presented; 2 500 L/kg for bottom dwelling fish, 250 for plankton feeding species and 50 for piscivorous species. As it is mainly piscivorous species that are consumed by humans a best estimate of 100 is selected.

25) The best estimate and range are defined in Bergström and Nordlinder /1992/. The amount of data concerning bioaccumulation of curium is scarce. Eyman and Trabalka /1980/ recommends bioaccumulation factors related to the trophic level of the fish species; 50 L/kg for piscivorous fishes and 250 for plankton feeding species. As it is mainly piscivorous species that are consumed by humans a best estimate of 50 is selected.

Table 8-10. Selected data for parameters related to the production of food for cattle and humans

Parameter	Unit	Best estimate	Min – Max	Distr function	Reference
Production of water plants (coast and lake)	kg/m^2/year	0.3	0.1 – 0.5	T	1
Yield of pasturage	kg d.w./m^2/year	0.5	0.4 – 0.6	T	Haak, 1983
Yield of cereals	kg d.w./m^2/year	0.5	0.4 – 0.6	T	2
Yield of root crops	kg d.w./m^2/year	2.3	1.8 – 2.8	T	3
Yield of vegetables	kg d.w./m^2/year	2	1.5 – 4	T	4
Irrigated area, garden plot	m^2	200	150-250	T	5
Irrigation events, garden plot	per year	10	6 – 14	T	6
Water per irrigation event	m^3/m^2	0.030	0.014 – 0.067	T(log)	7
Irrigation period	part of year	0.21	0.17 – 0.25	T	8

1) Data for the annual production of plants on the shores of the Baltic Sea were not available. Instead the production value for pasturage in the region is set as the maximum level. The primary production of macrophytes in the Model Area given in Kumblad /1999/ is used as a minimum value since the production of plants growing on the shores are larger than the production of these species off shore. In lack of data the same values as for the coastal model are selected.

2) The mean value selected is based on reported standard norm harvests for Uppsala county 1998 /SCB, 1999/. The mean value for 5 crops 1998 was 0.474 kg dw/m^2·year which was rounded to 0.5. The range is set to include the inter-annual variations given, i.e. up to 10-15 %.

3) No information on yield sizes of potatoes was found for Uppsala county. Standard yields were however calculated for the area 1998 /SCB, 1999/. This value is selected with about 20 % variation. The yield of carrots is higher per surface area, but the total production is considerably lower, about 10 % of that for potatoes. In addition much of carrots are used as fodder and not for human consumption.

4) The selected values are from 1996 /SCB, 1999/. The mean value is for lettuce (1.9 kg dw/m^2·year rounded to 2 kg dw/m^2·year). The range is set to include the values for cauliflower (about 1.5 kg dw/m^2·year) and white cabbage (about 4 kg dw/m^2·year).

5) This area should be of sufficient size to produce the annual amount of foodstuff for a family. The doses are not dependent on the size of this area as it is the amount of irrigation water per m^2 which is important for the exposure to humans from agricultural products.

6) A number of 10 irrigation events per year equals about one irrigation event per week during the summer period when garden plots are in use. A quite wide range is set since the number of events varies with crop as well as prevailing weather conditions.

7) In lack of data the same amounts as for an agricultural field is selected: According to Linner, Harry (Swedish University of agricultural sciences (SLU), personal communication, 1997) the annual water amount used for irrigation of agricultural fields is about 0.15 m^3/m^2. In Bergström *et al.* /1999/ this value was given a range of 0.1 to 0.2 m^3/m^2. Assuming that the number of irrigation events per year is 5 (3-7) the water amount used at each irrigation occasion is 0.030 m^3/m^2 varying from 0.014 m^3/m^2 (0.1 m^3/m^2/7 times) and 0.067 m^3/m^2 (0.2 m^3/m^2/3 times).

8) Cultivation in garden plots takes place during the summer months (second part of May, June, July and the first part of August) and irrigation is assumed to take place during the whole time. A maximum irrigation period of 90 days per year is therefore selected and a minimum of 2 months.

Table 8-11. Selected data for parameters related to the intake of radionuclides by cattle and humans via ingestion and inhalation.

Parameter	Unit	Best estimate	Min – Max/ Std	Distr function	Reference
Cattle					
Water consumption	l/day	70	65 – 75	T	1
Consumption of pasturage/water plants	kg d.w./day	8.5	8 – 9	T	2
Consumption of cereals	kg/day	11	10 – 12	T	3
Soil consumption	kg/day	0.3	0.15 – 0.5	T	4
Transpiration of water plants	g/m^2/hour	100	50 – 300	T(log)	Jörgensen *et al.* /1991/
Average time for water plant transpiration before consumption	days/year	100	80 – 120	T	5
Shore grazing period	days/year	30	20 – 40	T	6
Humans					
Water consumption	l/year	600	10 %	N	Bergström and Nordlinder /1990b/
Milk consumption	l/year	300	10 %	N	7,8
Meat consumption	kg/year	70	10 %	N	7
Vegetable consumption	kg/year	60	10 %	N	7
Root crop/potatoes consumption	kg/year	70	10 %	N	Bergström and Nordlinder /1990b/
Cereals consumption	kg/year	80	10 %	N	Bergström and Nordlinder /1990b/
Soil consumption	kg/year	0.1	10 %	N	9
Fish consumption	kg/year	30	10 %	N	Bergström and Nordlinder /1990b/
Inhalation rate	m^3/h	1	0.8 – 1.2	T	ICRP /1974/
Time of exposure to contaminated soil or contaminated air	hour/year	100	50 – 150	T	10

1) Torbjörn Morén, Swedish University of Agricultural Sciences in Uppsala (pers comm.). The values given are for dairy cows, water consumption of beef cattle are much lower (20-60 l/day).
2) According to Torbjörn Morén (see above) cattle need 8-9 kg food (in dry weight) each day together with the concentrated food.
3) According to Torbjörn Morén (see above) milk producing cattle consume 10 to 12 kg of concentrated food each day during the producing period (6 to 7 months per year). To assume that this amount is consumed during the whole year is a somewhat conservative assumption.
4) The consumption of soil adhering to "plant food" was calculated by Davis *et al.* /1993/ and the value here is extracted from that study. A relatively wide parameter range is set because of the difficulties to verify such data.
5) It is here assumed that the plant transpiration starts early in the year when light gets more abundant, i.e. in March and that outdoor grazing for cattle starts in May or June. It is not possible to verify these data within this study so a relatively wide parameter range (20 %) is selected.
6) Part of the time which cattle spend outdoors are assumed to be spent near shores of a coastal bay, a lake or a watercourse. During the remaining time it is assumed that grazing occurs elsewhere. A relatively wide parameter range is selected since this varies a lot depending on e.g. the shore line length and the production of shore plants.
7) Information from the Swedish Board of Agriculture (www.sjv.se) September, 2000.
8) This parameter value includes the consumption of all milk products, e.g. milk, cheese and butter. According to the Swedish Board of Agriculture the average consumption of milk and cheese for adults in Sweden is 115 l/year and 16.5 kg/year respectively. According to Arla (Swedish milk producers) (www.arla.se) it takes 10 l of milk to produce 1 kg cheese.
9) Extracted from Davis *et al.* /1993/.
10) Values estimated for work with soil i.e. agricultural practices. The range selected is relatively wide as such information is hard to evaluate.

Table 8-12. Selected data for parameters used to calculate the intake of radionuclides via inhalation of exhaust gases from peat combustion.

Parameter	Unit	Best estimate	Min – Max	Distr function	Reference
Fuel load	kg d.w./s	$1.0 \cdot 10^{-4}$	$(0.5 - 2.0) \cdot 10^{-4}$	T	1
Exposure time	hour/year	8000	6500 – 8760	T	2

1) This parameter gives the amount of peat combusted per time unit. An average value for energy content in peat is 22 MJ/kg /R Samuelsson, Swedish University of Agricultural Sciences in Umeå, pers. comm./. In general 20 000 kWh/year is used for heating of a family-house (pers. experience). If distributing this evenly over the year, about 0.4 kg peat is used per hour. This value is selected as a mean value. The minimum value is set to half of that and the upper to twice the mean value.

2) In lack of better data very conservative parameter values and a relatively wide range are selected.

Table 8-13. Half-lives /Firestone et al., 1999/ and dose coefficients for ingestion, inhalation and external exposure (ingestion and inhalation from EU /1996/ and external exposure from Svensson /1979/).

Nuclide	Type of dominating decay	Half life Year	Ingestion Sv/Bq	Inhalation Sv/Bq	External exposure $(Sv/h)/(Bq/m^3)$
H-3	β	12	$1.8 \cdot 10^{-11}$	$2.6 \cdot 10^{-10}$	0
C-14	β	5 730	$5.8 \cdot 10^{-10}$	$5.8 \cdot 10^{-9}$	0
Cl-36	β	301 000	$9.3 \cdot 10^{-10}$	$7.3 \cdot 10^{-9}$	0
Co-60	β, γ	5.3	$3.4 \cdot 10^{-9}$	$3.1 \cdot 10^{-8}$	$2.8 \cdot 10^{-13}$
Ni-59	β	76 000	$6.3 \cdot 10^{-11}$	$4.4 \cdot 10^{-10}$	0
Ni-63	β	96	$1.5 \cdot 10^{-10}$	$1.3 \cdot 10^{-9}$	0
Se-79	β	1 130 000	$2.9 \cdot 10^{-9}$	$6.8 \cdot 10^{-9}$	0
Sr-90	β	29	$2.8 \cdot 10^{-8}$	$1.6 \cdot 10^{-7}$	0
Zr-93	β	1 530 000	$1.1 \cdot 10^{-9}$	$2.5 \cdot 10^{-8}$	0
Nb-93m	γ	16.1	$1.2 \cdot 10^{-10}$	$1.8 \cdot 10^{-9}$	$5.5 \cdot 10^{-17}$
Nb-94	β, γ	20 300	$1.7 \cdot 10^{-9}$	$4.9 \cdot 10^{-8}$	$1.6 \cdot 10^{-13}$
Mo-93	EC	3 500	$3.1 \cdot 10^{-9}$	$2.3 \cdot 10^{-9}$	0
Tc-99	β	211 000	$6.4 \cdot 10^{-10}$	$1.3 \cdot 10^{-8}$	0
Pd-107	β	6 500 000	$3.7 \cdot 10^{-11}$	$5.9 \cdot 10^{-10}$	0
Ag-108m	γ	418	$2.3 \cdot 10^{-9}$	$3.7 \cdot 10^{-8}$	$1.6 \cdot 10^{-13}$
Cd-113m	β	14.1	$2.3 \cdot 10^{-8}$	1.1E-07	0
Sn-126	β, γ	100 000	$4.7 \cdot 10^{-9}$	$2.8 \cdot 10^{-8}$	$3.0 \cdot 10^{-15}$
I-129	β	15 700 000	$1.1 \cdot 10^{-7}$	$3.6 \cdot 10^{-8}$	$3.4 \cdot 10^{-16}$
Cs-135	β	2 300 000	$2.0 \cdot 10^{-9}$	$8.6 \cdot 10^{-9}$	0
Cs-137	β, γ	30	$1.3 \cdot 10^{-8}$	$3.9 \cdot 10^{-8}$	$5.6 \cdot 10^{-14}$
Sm-151	β	90	$9.8 \cdot 10^{-11}$	$4.0 \cdot 10^{-9}$	$4.6 \cdot 10^{-18}$
Eu-152	β, EC	14	$1.4 \cdot 10^{-9}$	$4.2 \cdot 10^{-8}$	$1.5 \cdot 10^{-13}$
Eu-154	β, EC	8.6	$2.0 \cdot 10^{-9}$	$5.3 \cdot 10^{-8}$	$1.3 \cdot 10^{-13}$
Ho-166m	γ	1 200	$2.0 \cdot 10^{-9}$	$1.2 \cdot 10^{-7}$	$1.6 \cdot 10^{-13}$
U-232	α	69	$3.3 \cdot 10^{-7}$	$3.7 \cdot 10^{-5}$	$1.6 \cdot 10^{-13}$
Pu-238	α	88	$2.3 \cdot 10^{-7}$	$1.1 \cdot 10^{-4}$	$1.3 \cdot 10^{-17}$
Pu-239	α	24 000	$2.5 \cdot 10^{-7}$	$1.2 \cdot 10^{-4}$	$6.6 \cdot 10^{-18}$
Pu-240	α	6 563	$2.5 \cdot 10^{-7}$	$1.2 \cdot 10^{-4}$	0
Pu-242	α	380 000	$2.4 \cdot 10^{-7}$	$1.1 \cdot 10^{-4}$	0
Am-241	α	432	$2.0 \cdot 10^{-7}$	$9.6 \cdot 10^{-5}$	$1.1 \cdot 10^{-15}$
Cm-243	α, EC	29	$1.5 \cdot 10^{-7}$	$6.9 \cdot 10^{-5}$	$1.0 \cdot 10^{-14}$

8.5 Evaluation of data and uncertainties

The *geometric data* used in the coastal model are connected with the least uncertainties as they describe the situation of today, which has been investigated. For such data in the other models, results from models predicting the future evolution has been used and the uncertainties increase.

Comparing geometrical parameters with *physical/chemical and biological parameters* for all models it is clear that data for the former to a much larger extent is site-specific and therefore are given narrower distributions. The physical/chemical and biological ones are, with some exceptions, generic but the ranges are set up so that they should include the reasonable values describing the conditions in the area today as well as in the future.

Data about *living habits of humans and cattle* represent the situation in Sweden of today. How this will change in a far future (up to 10 000 years from now) can not be given for sure, but in a reasonable time period we think that the values chosen will be relevant.

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