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SR 97

Data and data uncertainties

Compilation of data and data uncertainties for radionuclide transport calculations

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Preface

The present report is written in support of the quantitative assessment calculations within the SR 97 project. The production of the report has to a large extent implied compiling and evaluating technical reports from a wide range of technical disciplines. The main evidence of the realism and pessimism in parameter values given in this report can only be found in these underlying reports. I have, however, tried to evaluate the reasoning in the different underlying reports in search of logical arguments for the parameters selected. Clearly, the authors of the underlying reports are not responsible for potential misunderstandings or mis-interpretations of their work. It must finally be stated that the production of this report would have been impossible without lengthy discussions with the SKB scientific staff. In particular I wish to mention Allan Hedin, Patrik Sellin, Jan-Olof Selroos and Ulrik Kautsky, who helped me out at numerous occasions.

Johan Andersson

Abstract

This report concerns integration of data and data uncertainties in the radionuclide transport calculations within the SR 97 project. More specifically the present report:

- establishes a framework for handling data uncertainty within SR 97,
- explores uncertainties in the different underlying analyses and information such as inventory, canister life time, solubilities, K_d-vales, or different flow related migration parameters, which provide input to the radionuclide release and transport models used,
- suggests and motivates ”reasonable” input values, and ”pessimistic” input values representing conditions at Aberg (Äspö), Beberg (Finnsjön) and Ceberg (Gideå) when applicable, for the different models used,
- suggests ”probabilistic” parameter distributions when underlying data support any distribution.

The intention of presenting ”*reasonable*” estimates is one of illustration - to obtain a view on how the repository system would operate without making overly optimistic or pessimistic assumptions. A *pessimistic* input datum implies a selection of a parameter value (and conceptual model) within the uncertainty range, which maximises the consequence.

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Summary and conclusions

This report concerns compilation of data and evaluation of uncertainties in these data for the radionuclide transport calculations within the SR 97 project. More specifically the present report:

- establishes a framework for handling data uncertainty within SR 97,
- explores data uncertainties in the different underlying analyses which provide input to the radionuclide release and transport models used to explore the radiological consequences of the SR 97 canister defect scenario,
- suggests and motivates ”reasonable” input values, and “pessimistic” input values representing conditions at Aberg (Äspö), Beberg (Finnsjön) and Ceberg (Gideå), when applicable, for the different models used,
- suggests ”probabilistic” parameter distributions when exist underlying data support any distribution.

The uncertainty evaluation concentrates on the quantitative models or analyses selected for the model chain. The issue of conceptual model uncertainty is partly included in this evaluation, whereas the more fundamental questions concerning model selection and which potential model couplings to analyse are not addressed here. These latter questions are discussed in the main SR 97 report, directly, or in underlying reports referred to in the main SR 97 report.

The intention of presenting a ”*reasonable value*” is to obtain a view on how the repository system would operate without making overly optimistic or pessimistic assumptions. The reasonable value is selected for illustration. The pragmatic approach adopted here is that a reasonable value should be based on model analyses or direct measurements, which are:

- plausible building on the present understanding of the phenomenon, where processes known (or generally thought) to be involved 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.

One way of bounding the impact of uncertainty is 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.

Basing the performance assessment only on “reasonable” or on “*pessimistic*” parameter values may give a quite misleading picture of the actual performance of the repository, in particular if the results of the reasonable analysis and the pessimistic analysis deviate

very much. As already mentioned, the reasonable case is judgmental and even if it may represent the most plausible conditions there may be many other, and strongly deviating, conditions that are almost as plausible. In contrast, combing all pessimistic parameter values into a single case would lead to totally unrealistic estimates of performance. These problems could ideally be handled by analysing the *probability distributions* of the performance parameters, which then could be used to estimate a probability distribution of the radiological consequences. In discussing probabilistic estimates, assessing the potential correlation between parameters is of key importance. Neglecting correlation may grossly underestimate the likelihood of certain outcomes. However, given the difficulties in estimating probability distributions (and the inter-parameter correlation) the present report only suggests probability distributions in case there is any evidence for such distributions. In other cases, the report in qualitative terms discusses the potential correlation with other parameters.

The calculation chain and the information flow

The near-field source term model COMP23, the far-field migration code FARF31 and the code BIO42 perform the direct radionuclide transport analyses in SR 97. The various sources of information to these codes build on elaborate modelling combined with data analysis, see figure 1.

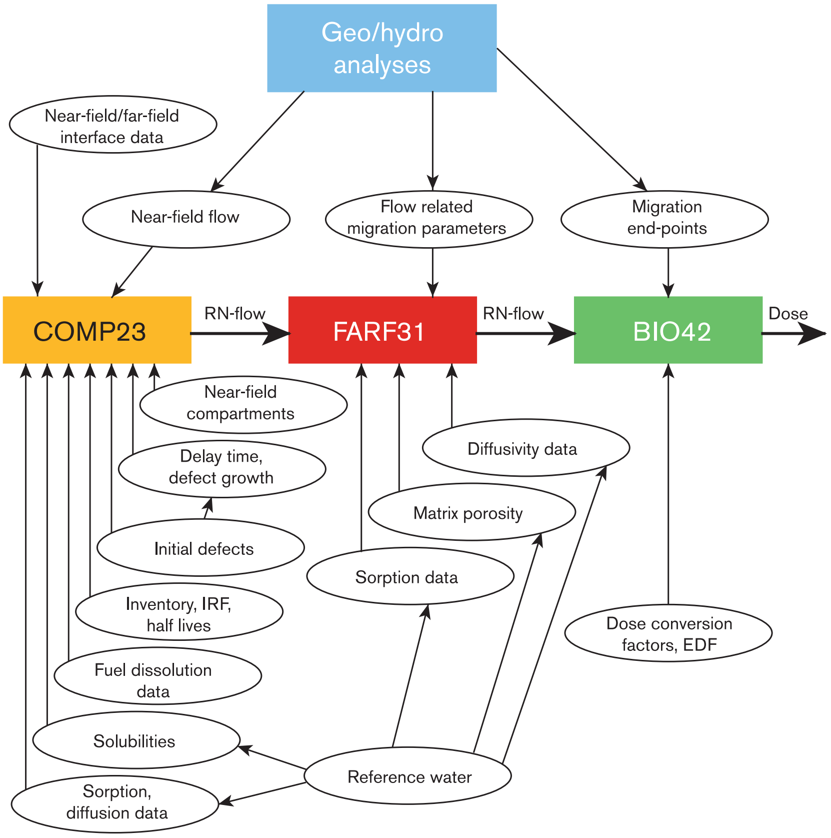


Figure 1. The chain of models used for evaluating radiological consequences and the primary sources of information for these models.

Most of the information compiled and evaluated in this report has been obtained from a number of underlying reports presenting data for the SR 97 analysis. To facilitate a systematic treatment of uncertainties a common template was used for the discussion of uncertainties in many of the underlying reports.

Inventory

The total initial inventories, at disposal, for the fuel pellets and the metal parts are directly used as input in the near-field code. The fuel composition is constrained by the heat load and the space available in the canister, which limits the variability of the possible inventory in a canister. It is suggested that the *reasonable* inventory should be based on the inventory calculated by Håkansson (1998) for 12 BWR fuel elements with a burn-up of 38 MWd/ kg U. No pessimistic case is suggested.

Radionuclide release from the spent fuel

The source term heavily depends on the dissolution of the radionuclides in the spent fuel. The dissolution models used in the near-field model COMP23 (Romero, 1995) includes the following mechanisms:

1. immediate dissolution of a certain fraction of the inventory specified for each nuclide (IRF or instant release fraction),

2. release of the radionuclides contained in the UO_2 matrix at a rate R equal to the rate of the dissolution/conversion of the uranium dioxide matrix.

A refined fuel conversion model, based on dissolution experiments with spent fuel in reducing environments, attempts at a realistic description of the fuel oxidation and resulting dissolution rate. This model implies a dissolution rate of $R=10^{-8}$ yr^{-1}, which consequently could be taken as a *reasonable value.* It is not really possible to suggest a *pessimistic* fuel conversion rate. Instead it is suggested to only provide the reasonable value for calculations and then only discuss possible implications of the uncertainty of the dissolution rate.

Reasonable values of the instant release fraction (IRF) for the different radionuclides in the spent fuel are estimated from measurements of fission gas releases from representative Swedish BWR fuel combined with information from leaching studies on LWR and CANDU fuel. Pessimistic values are estimated from the highest values found in these experiments.

Canister defects and delay time

The canister will be designed such that it will fully isolate the waste and such that no known corrosion process would lead to a failure before 100 000 years. A remaining possibility for canister failure would, however, be a development of initial defects not discovered in the quality control. The most likely position of such a defect would be at the weld of the lid. It is suggested that the maximum defect height would not exceed 1µm. One may further assume that this defect extends half a circumference, i.e. approximately 1m. This results in a defect size of about 1 mm^2. Even if the risk of not detecting such a defect is close to zero, it is pessimistically suggested that (at most) 0.1% of the canisters could have such a defect.

The defect grows when the corrosion products resulting from the corrosion of the steel vessel eventually will strain the copper vessel. With a realistic estimate of the iron corrosion rate (0.1 µm/year) a large damage will not occur before $2 \cdot 10^5$ years and before this time the defect size is almost unchanged. For a very pessimistic estimate of the corrosion rate (1.0 µm/year) the damage will not occur before 22 000 years. These two failure times are used as reasonable and pessimistic estimates respectively.

Radionuclides may migrate from the failed canister also in when there is a small defect, but migration cannot start before there is a continuous path between the fuel rods and the defect. The time it takes for development of such a path is called the delay time. The delay time is controlled by the bentonite permeability, the size of the defect, but also by the development of a gas overpressure due to the corrosion, which will resist the water flow. Results of modelling water inflow combined with hydrogen formation due to corrosion for a 1 mm^2 circular defect suggest a delay time of $2 \cdot 10^5$ years. This time is taken as a *reasonable* estimate However, one may pessimistically assume that the gas pressure inside the canister would not build up sufficiently fast to control the water inflow and that the defect has another shape. Accounting for uncertainties in bentonite hydraulic conductivity and in the shape of the defect would then imply a very *pessimistic delay time* of 300 years.

Groundwater composition - Reference waters

Reference waters for SR 97 are taken from the groundwater chemical composition measurements at depth in four different boreholes selected to represent Aberg, Beberg and Ceberg. Using a principal component analysis and a qualitative discussion of the past hydrogeologic history of the sites it is suggested that these waters can be described in terms of mixing portions of e.g. meteoric water, biogenic water, sea water and brine groundwater. The *reasonable* water compositions are obviously the reference water chemistries provided for the different sites. Given the spatial variability and the uncertainty in water composition it seems reasonable to represent the uncertainty and the spatial variability in water composition by the range in water composition represented by the four reference waters. The chemical composition of the groundwater affects performance parameters such as solubility and sorption in different ways, which makes it impossible to directly nominate a *pessimistic* water composition. Instead the approach suggested is to select the composition in the range of reference waters and buffer pore water, which will produce the most pessimistic solubility, diffusivity or sorption coefficients.

Solubilities

Solubility calculations are made for the Aberg, Beberg and Ceberg reference waters and for a bentonite water using the speciation code EQ3NR. The uncertainties associated with co-precipitation and selection of solubility controlling solid phases makes it necessary to select the phases leading to the highest solubility also for the reasonable solubility. The suggested *pessimistic case* is obtained by selecting the highest solubility of each element regardless of the consistency in water chemistry.

Sorption and diffusivity in bentonite

SR 97 models migration through the buffer by diffusion and sorption. The near-field release code COMP23 describes these processes with element specific values for the distribution coefficients, K_d, the effective diffusivity D_e, and porosity ε. For most elements porosity is given by the bentonite specification, but some elements require a lower porosity in order to handle ion exclusion. Evaluation of published measurements (diffusion and sorption properties in water-saturated compacted bentonite) and critically reviewing sources of errors provide reasonable values, pessimistic values and ranges of the assessment parameters.

Sorption and diffusivity in backfill

SR 97 models migration through the backfill (a 15% bentonite / 85% crushed rock mixture) by diffusion and sorption, i.e. the same as in the buffer. The K_d values suggested result from a proportional contribution of 15% of the bentonite values and 85% of the rock values.

Matrix porosity and diffusivity

Matrix porosity and diffusivity are used in the far-field migration code FARF31 to describe diffusion in the rock matrix. The model assumes that there exists an interconnected pore space inside the rock matrix and models migration as a diffusion process retarded by sorption on the rock matrix itself. Data are estimated using diffusion experiments with tritiated water (HTO) and some cat-ions in salty water in rock samples from Äspö (i.e. Aberg). Diffusivities for other nuclides are assessed from their theoretical relation to the HTO diffusivity by considering differences in free water diffusivities and possibilities for anion exclusions or surface diffusion. Reasonable parameters are obtained by considering all these effects, whereas the pessimistic values omits (uncertain) effects leading to high diffusivities and are based on pessimistic water compositions.

Geosphere sorption

The far-field migration code FARF31 models sorption inside the rock matrix as a linear process through the use of distribution factors (K_d). Sorption data in terms of K_d values are obtained by exploring different experimental databases, while considering the water chemistry at the different sites. Within this range of water chemistries, salinity has the largest impact on the K_d-values. The *reasonable* sorption coefficients to use in SR 97 are taken from the reasonable values as suggested by these studies. To be consistent with water chemistries one should use ”saline” values for Aberg and ”non-saline” values for Beberg and Ceberg. A clearly *pessimistic* selection of sorption coefficients is to select the lowest K_d found in the studies. However, for Ceberg it appears evident that non-saline conditions will prevail for the base case and initial canister defect scenario. Consequently, the lowest fresh water values could be used for Ceberg.

Groundwater flow

Groundwater flow affects radionuclide release and migration in several ways. It affects near field release, migration through the geosphere and the distribution of discharge into the biosphere. A hydrogeological model of a site requires input from a geological structure model and specific hydrogeologic data. For practical reasons the hydrogeologic models are divided into a regional model and a more detailed site scale model.

The geological structure models are based on various sources of information including topography, direct observations such as outcrop and core mapping and indirect data such as geophysical measurement. The wealth of data varies between the sites as well as the approaches to interpretation. In addition to *reasonable* structure models for SR 97 sites, the data analysis provides input to variant interpretations in the form of potential additional structures. It is not possible to select a *pessimistic* structure model. The approach rather has to be to study the implications of alternative structure models in order to explore whether any of the possible alternatives would lead to less favourable performance than the reasonable structure model.

Existing data and descriptions are compiled for use in the hydrogeologic modelling of the Aberg, Beberg and Ceberg sites. The interpretation of the data allows for the identification of different variants of data sets to be used. The underlying conceptual model of the rock assumed is one of a rock domain described as a spatially varying stochastic continuum intersected by conductor domains (fracture zones), also modelled as porous media, but of hydraulic properties distinct from the rock domain. The approach further assumes a nested approach using a site scale model with relatively much detail in conductive structures and adoption of a stochastic continuum model embedded in a regional scale model with less geometrical detail and with equivalent, i.e. non-stochastic, hydraulic parameters. In addition, discrete fracture network and channel network modelling are used in a few cases as alternative means of modelling the hydraulics in site scale.

Various results of the flow modelling are used in the modelling of the radio-nuclide near-field, far-field and biosphere transport, as described below.

Flow related migration parameters - near field

The near-field code COMP23 calculates the non-stationary nuclide transport in the near field of a repository. Radionuclides leaking out from the canister will diffuse through the buffer and through various pathways migrate into the flowing water in the rock fractures. The prime flow related input parameter is the groundwater flow (darcy velocity) in the canister scale. This information is obtained from the site scale stochastic continuum groundwater flow simulations, complemented by analyses considering the flow paths to be represented by discrete fractures. The reasonable value is taken from the median of the ensemble of the stochastic continuum results, whereas the pessimistic case is taken from the 95%-tile of the variant with the highest local darcy velocity. However, the difference between different variants is low, most of the spread of darcy velocity is due to spatial variability within a realisation.

Flow related migration parameters - far-field

Far-field transport is modelled using a streamtube approach where particle ”travel times”, and discharge locations of a set of one-dimensional streamtubes are obtained from particle tracking in the site scale flow model. The specific one-dimensional transport code used, FARF31, incorporates advection and dispersion along the migration path, matrix diffusion combined with sorption in the rock matrix and chain decay. To a large extent, the retention properties depend on the “migration resistance”. This can be expressed as the quotient (a_rL/q) between the ”flow wetted surface per volume of rock” (a_r) times the migration path length (L) and the darcy velocity (q), or using other parameters, the product (t_wa_w) between water ”transit time” (t_w) and “flow wetted surface per volume of water” (a_w). The result of the site scale stochastic continuum groundwater flow simulations is also the main source of flow information. In addition, estimates of the flow wetted surface and some related parameters are suggested, based on site specific information from a few tracer tests, geological characterisation, hydraulic measurements, and modelling. The flow wetted surface estimates are based on estimates of the conductive fracture frequency, which in turn is estimated from the hydraulic tests. Several assumptions are needed in order to handle the lack of adequate data for some of the parameters. The reasonable “transit-time” is taken from the median of the base case of the stochastic continuum results, whereas the pessimistic case is taken from the 5%-tile values from the stochastic continuum variant with the shortest “time”. In addition, pessimistic values of the flow wetted surface are a factor of ten lower than the reasonable value. It is ensured that the combination of “transit time” and “flow wetted surface” represent the desired “migration resistance”.

Biosphere

The biosphere modelling aims at describing the transfer of radionuclides in the biosphere in order to make it possible to estimate radiological consequences for exposed groups (man) and the environment from radionuclide releases into the biosphere. Each site is first divided into different ecosystem type *modules* and then *ecosystem specific dose conversion factors* (EDFs) are calculated in each such module. In the final assessment, the BIO42 code in the calculation chain selects a module based on the predicted recharge point in the far-field assessment and calculates doses (Sv/yr) by multiplying the release from the far-field (in terms of Bq/yr) with the EDFs (Sv/Bq) of the selected module. The modules currently available are *well, lake, running water, coast, soil* and *peat*.

Sensitivity analyses suggest that the range of uncertainty, if the release is known to be to a specified module, typically is around two orders of magnitude. However, the module selection has an even greater impact - the difference between a module with high dilution (open coast) and one with little dilution (well or peat) is many orders of magnitude. The reasonable value is based on the module suggested by the discharge areas of the hydrogeological modelling. For the pessimistic estimate it is suggested that the releases reach the biosphere module leading to highest dose rates (i.e. usually the soil, peat or well module).

Sammanfattning och slutsatser

Denna rapport sammanställer de data och utvärderar osäkerheter i dessa data som ska användas för beräkningar av radionuklidtransport i SR 97. Rapporten

- etablerar en struktur för hur dataosäkerhet hanteras inom SR 97,
- utvärderar dataosäkerheter i de olika underliggande analyser som i sin tur ger indata till de modeller av frigörelse och transport av radionuklider som används för att analysera de radiologiska konsekvenserna av kapseldefektscenariot i SR 97,
- föreslår och motiverar ”rimliga” och försvarbara ”pessimistiska” indata till modellerna, representerande förhållanden vid Aberg (Äspö), Beberg (Finnsjön) och Ceberg (Gideå) (när detta är aktuellt),
- föreslår ”probabilistiska” fördelningar för de indata där det finns underlag för att kunna föreslå sådana fördelningar.

Osäkerhetsvärderingen fokuserar på de modeller och analyser som ingår i den s.k. ”modellkedjan” (se nedan). Konceptuell osäkerhet behandlas delvis, men de mer fundamentala frågorna om vilka modeller som bör användas och vilka modellkopplingar som behöver beaktas behandlas inte. Dessa senare frågeställningar behandlas dels direkt i Huvudrapporten till SR 97 och dels i den s.k. ”Processrapporten” som tas fram som ett underlag till SR 97.

Syftet med att ta fram en ”*rimlig uppskattning*” är att kunna beskriva hur förvarssystemet förväntas fungera utan att man gör överdrivet optimistiska eller pessimistiska antaganden. Den rimliga uppskattningen är en illustration och det finns inget korrekt svar på vad som menas med begreppet. Den pragmatiska ansats som används i rapporten är att den rimliga uppskattningen av en parameter skall kunna härledas från en modell eller en direkt mätning som:

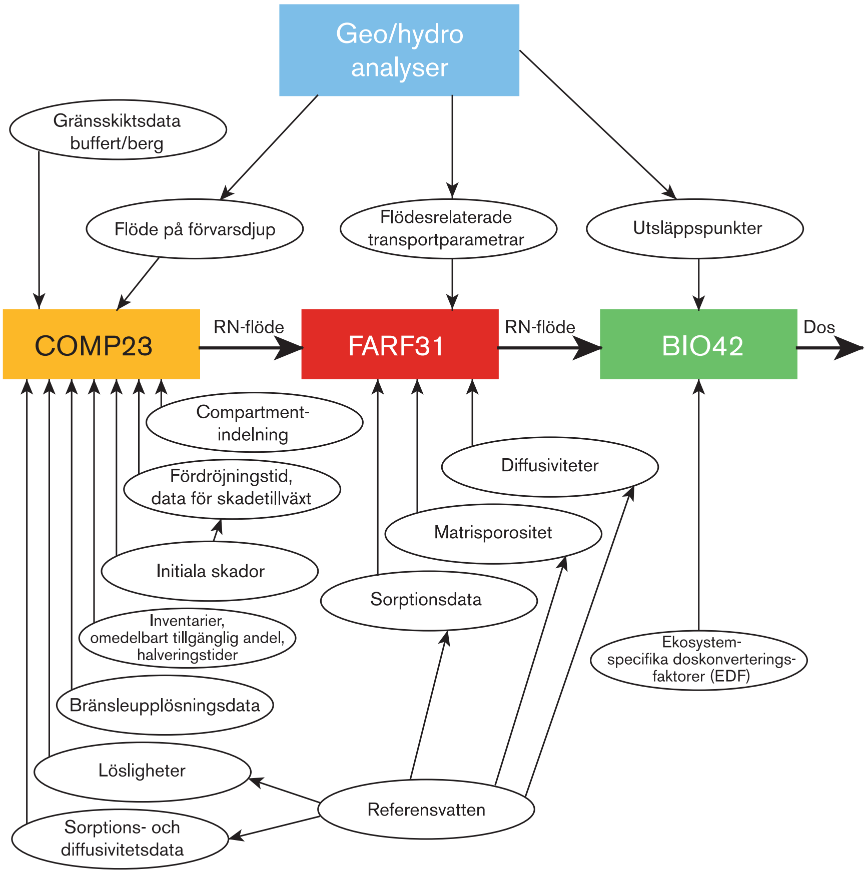
- på ett trovärdigt sätt bygger på vår nuvarande kunskap om fenomenet och där processer som man vet (eller allmänt antar) påverkar ingår i analysen,
- baseras på tillgängliga data när sådana finns,
- är konsistent, dvs. samtidigt tar hänsyn till de parametrar som beror på varandra och så att den rimliga uppskattningen av dessa parametervärden inte innebär en orimlig kombination av data.

En övre gräns för inverkan av osäkerheterna i indata är att välja ”*pessimistiska*” indata. P*essimistiskt* indata innebär att man väljer parametervärde (och konceptuell modell) inom osäkerhetsintervallet, som maximerar konsekvensen.

Om säkerhetsanalysen enbart baseras på analys av ”rimliga” eller ”pessimistiska” indata kan detta leda till en missvisande bild av hur förvaret faktiskt kommer att fungera. Detta gäller speciellt om de rimliga och pessimistiska värdena skiljer sig mycket från varandra. Det är en bedömningsfråga vad som kan betraktas som en rimlig uppskattning. Även om den representerar trovärdiga förhållanden kan det finnas andra, starkt avvikande, förhållanden som är nästan lika troliga. De pessimistiska värdena kan, å andra sidan, visa sig vara orealistiskt pessimistiska. Idealt skulle man kunna hantera dessa problem genom att göra en samlad riskbedömning där fördelningen av osäkerheter för de olika parametrarna vägs in. Det är dock inte alltid möjligt att på ett meningsfullt sätt skatta sannolikhetsfördelningar för alla parametrar. Om man gör en sådan probabilistisk riskanalys är det vidare nödvändigt att beakta korrelationen mellan de ingående parametrarna. Försummas denna skulle det kunna leda till att sannolikheten av olika kombinerade fall underskattas. Denna rapport begränsas därmed till att beskriva kända korrelationer och till att skatta fördelningar för de parametrar där det finns information som kan användas för att skatta fördelningen.

Beräkningskedjan och flödet av information

Beräkningskedjan består av de datormodeller som direkt används för att beräkna radionuklidtransport för olika fall. Den består av källtermsmodellen (närområdesmodellen) COMP23, fjärrområdestransportmodellen FARF31 och dosmodellen BIO42. Indata till dessa modeller kommer i sin tur från olika mer eller mindre komplexa modellberäkningar eller dataanalyser av olika förhållanden eller fenomen, se figur 1.



Figur 1. Kedjan av modeller som används för att beräkna radionuklidtransport samt de primära källorna till indata för dessa modeller.

Den mesta informationen som samlats och utvärderats i denna rapport har erhållits från ett stort antal underlagsrapporter som presenterar data att använda i SR 97 analysen. I regel innehåller dessa underlagsrapporter en osäkerhetsdiskussion. För att förenkla en systematisk utvärderingen av osäkerheterna disponeras diskussionen om osäkerheter på ett likartat (gemensamt) sätt i många av dessa underlagsrapporter.

Inventarium

Källtermsmodellen behöver information om inventariet vid deponering av radionuklider i bränslekutsar och metalldelar hos det använda bränslet. För en enskild kapsel begränsas sammansättningen av de använda bränslet av att den totala värmelasten inte får överstiga vissa värden och av utrymmet i kapseln. Detta begränsar skillnaden i inventarium mellan olika kapslar. En bästa uppskattning av inventariet ges av en beräkning genomförd av Håkansson (1998) för 12 BWR bränsleelement med en utbränningsgrad av 38 MWd/ kg U. Det är inte meningsfullt att ange något pessimistiskt fall.

Radionuklidfrigörelse från det använda bränslet

Källtermen beror i hög grad av upplösningen av radionukliderna som finns i det använda bränslet. Följande frigörelsemekanismer kan behandlas i modellen COMP23 (Romero, 1995):

1. omedelbar upplösning av en viss fraktion av inventariet specifikt för varje nuklid (IRF eller ”instant release fraction”),

2. frigörelse av nuklider som finns inne i UO_2 matrisen med en hastighet R som motsvarar hastigheten för upplösning/omvandling av UO_2-matrisen.

En förfinad bränsleomvandlingsmodell har utvecklas, som baseras på upplösningsförsök med använt bränsle i reducerande miljö. Modellen anger en upplösningshastighet om $R=10^{-8}$ yr^{-1}, vilket därmed kan användas som *rimlig uppskattning*. Det är inte meningsfullt att ange någon *pessimistisk* omvandlingshastighet. Betydelsen av osäkerheten i omvandlingshastigheten får istället diskuteras kvalitativt i säkerhetsanalysen.

Rimliga uppskattningar av IRF för olika nuklider i det använda bränslet uppskattas från mätningar av frigörelse av fissionsgaser från representativt svenskt BWR bränsle, kombinerat med resultat från upplösningsförsök på LWR och CANDU bränsle. Pessimistiska värden uppskattas genom att välja de högsta värden på IRF som har funnits i dessa studier.

Kapselskador och fördröjningstid

Kapseln ska utformas så att den fullständigt isolerar avfallet och så att ingen känd korrosionsprocess ska leda till att bränslet exponeras. En kvarvarande möjlighet att erhålla en kapselskada är dock att det skulle kunna finnas en initial defekt som inte upptäcks vid kvalitetskontrollen av kapslar som skall deponeras. Det troligaste läget för en sådan effekt är i svetsfogen i kapselns lock. Man kan anta att defekten inte kan vara större än 1μm och att den maximalt omfattar en halv omkrets. Detta innebär en totalarea av 1 mm^2. Även om risken för att inte hitta en sådan defekt i kvalitetskontrollen måste bedömas som mycket liten ansätts pessimistiskt att (som mest) 0.1% av kapslarna har en sådan defekt.

Defekten växer när korrosionsprodukterna som bildas genom korrosion av stålinsatsen till slut kommer att deformera kopparhöljet. Med en realistisk uppskattning av järnets korrosionshastighet (0.1 μm/år) uppstår inte en stor skada förrän om $2 \cdot 10^5$ år. Innan dess är defektens storlek i det närmaste opåverkad. Med ett mycket pessimsitiskt antagande om korrosionshastigheten (1. μm/year) uppstår skadan efter 22 000 år. Dessa två skadetider anges som rimliga respektive pessimistiska uppskattningar.

Migrationen av radionuklider från en skadad kapsel kan ske även genom en den initiala defekten, men transporten kan inte börja förrän det finns en kontinuerlig vattenväg mellan defekten och bränslestavarna. Tiden som det tar för att skapa en sådan förbindelse kallas *fördröjningstid*. Fördröjningstiden beror på bentonitens permeabilitet, defektens storlek och form men också på det gasövertryck som bildas inne i kapseln på grund av korrosionen. Modellanalyser för ett cirkulärt hål om 1 mm^2 och som som tar hänsyn till gasens mottryck resulterar i en fördröjningtid av i storleksordningen $2 \cdot 10^5$ år. Detta värde anges som *rimligt*. Ett pessimistiskt värde om 300 år fördröjningstid fås om man försummar gasens mottryck och tar hänsyn till osäkerheter hos skadans form och bentonitens permeabilitet.

Grundvattnets sammansättning - Referensvatten

Mätningar av den kemiska sammansättningen för grundvatten från fyra olika borrhål utvalda att representera Aberg, Beberg och Ceberg, bildar referensvatten för SR 97. Utifrån en statistisk principalkomponentsanalys och en kvalitativ diskussion avseende den tidigare hydrogeologiska utvecklingen för de olika platserna föreslås det att dessa vatten kan beskrivas i termer av blandningar av t.ex. meteoriskt vatten, biologiskt påverkat vatten, havsvatten och djup liggande saltlösningar (”brine”). Den rimliga uppskattningen av framtida sammansättning är uppenbarligen den sammansättning grundvattnet idag har vid de olika platserna. Med tanke på den rumsliga variationen och framtida osäkerheter antas det rimligt att representera osäkerheten i framtida grundvattensammansättning med det värdeområde som ges av skillnaden mellan de fyra olika referensvattnen. Den kemiska sammansättningen påverkar funktionsparametrar, som löslighet och asbortionsförmåga, på olika sätt. Det är därför inte möjligt att ange en enskild sammansättning som mest pessimistisk. Detta hanteras istället genom att välja de mest pessimistiska värdena för lösligheter, diffusiviteter och sorptionsvärden som fortfarande är möjliga inom ramen för de olika uppmätta grundvattensammansättningarna.

Lösligheter

Med hjälp av specieringkoden EQ3NR beräknas lösligheter för olika specier i referensvattnen för Aberg, Beberg, Ceberg, och för ett speciellt bentonitvatten. De osäkerheter som finns beträffande medfällning och val av löslighetskontrollerande fast fas gör att det är nödvändigt att även som rimlig uppskattning välja den fas som leder till de högsta lösligheterna. De pessimistiska lösligheterna erhålls genom att, för respektive ämne, välja den högsta lösligheten som beräknats för någon av de olika vattensammansättningarna.

Sorption och diffusivitet i buffert

SR 97 beskriver transport genom bufferten med processerna difusion och sorption. Närområdeskoden COMP23 beskriver dessa processer med ämnesspecifika värden för fördelningsfaktorer, K_d, effektiv diffusivitet D_e, och porositet ε. För de flesta ämnen ges porositeten av bentonitens specifikation, men för vissa ämnen måste porositeten minskas för att kunna representera anjon exklusion. Rimlig uppskattning, pessimistiska värden och osäkerhetsintervall erhålls genom att utvärdera olika publicerade mätningar av diffusions- och sorptionsegenskaper i vattenmättad bentonit samt genom att kritiskt utvärdera olika felkällor.

Sorption och diffusivitet i återfyllnad

SR 97 beskriver transport genom återfyllnaden (en blandning av 15% bentonit och 85% bergkross) med difusion och sorption, dvs. samma processer som i bufferten. De föreslagna K_d värdena har tagits fram genom att proportionellt vikta med 15% av värdena i bentonit och med 85% av värdena i berg (geosfären).

Porositet och diffusivitet i bergmatrisen

Matrisporositet och diffusivitet används i fjärrområdestransportmodellen FARF31 för att beskriva difusion i bergmatrisen (det ”intakta berget”). Modellen utgår ifrån att det finns en sammanhängande porvolym inne i det intakta berget och beskriver transporten som en difusionsprocess retarderad genom sorption direkt på bergmatrisen. Data uppskattas från difusionsförsök, med tritierat vatten (HTO) och med några katjoner i salt vatten, utförda på bergmaterial från Äspö (dvs. Aberg). Diffusiviteter för andra ämnen erhålls genom att ta hänsyn till olika ämnens diffusivitet i fritt vatten och genom att ta hänsyn till möjligheterna för anjon-exklusion och för ytdiffusion. Den rimliga uppskattningen erhålls genom att ta hänsyn till alla dessa effekter, medan pessimistiska värden erhålls genom att inte ta hänsyn till (osäkra) processer som leder till höga diffusiviteter samt genom att konsekvent välja ofördelaktig vattenkemi.

Sorption i geosfären

Modellen för transport i fjärrområdet, FARF31, beskriver sorptionen inne bergmatrisen som en lineär process med hjälp av ämnesspecifika fördelningsfaktorer (K_d). Sorptionsdata i termer av K_d värden erhålls genom att utvärdera olika experimentella databaser och samtidigt ta hänsyn till grundvattnets kemiska sammansättning vid de olika platserna. Inom denna variationsbredd är det skillnader i salinitet som mest påverkar K_d-värdena. Rimlig uppskattning för SR 97 tas från den bästa uppskattning som erhållits vid dessa studier. Detta innebär att för Aberg används värden för salt vatten, medan för Beberg och Ceberg används värden för ”sött” vatten. Ett uppenbart pessimistiskt val av fördelningskoefficienter är att alltid välja de lägsta K_d värden som observerats, oberoende av vattenkemi. För Ceberg gäller dock att ”icke-salta” förhållanden kan anses gälla i framtiden för kapseldefektscenariot. Därmed väljs de lägsta icke-salina K_d-värdena som pessimistiskt fall för Ceberg.

Grundvattenströmning

Grundvattnets strömning påverkar frigörelse och transport av radionuklider på flera sätt. Den påverkar frigörelsen från närområdet, transporten genom geosfären och fördelningen av utströmningen i biosfären. En platsspecifik hydrogeologisk modell baseras på en geologisk modell av bergets sprickzoner och på specifika hydrogeologiska data. Av praktiska skäl delas de hydrogeologiska modellerna i SR 97 in i regionala modeller och platsskalemodeller. Platskalemodellen är inbäddad i den regionala modellen.

Modellen av sprickzoner baseras på data från olika informationskällor som topografi, direkta observationer av berg i dagen och borrkärnor, geofysiska mätningar m.m. Tillgången på data, liksom använd metodik för tolkning, varierar mellan de platser som studeras i SR 97. Förutom de sprickzoner som får anses representera en rimlig uppskattning av SR 97 platserna, ger dataanalysen underlag för alternativa tolkningar i form av ytterligare tänkbara sprickzoner. Det är inte möjligt att välja ut en pessimistisk modell av sprickzoner. Istället bör följderna av de olika alternativa modellerna studeras för att kunna utreda om något av de tänkbara alternativen skulle kunna leda till mindre fördelaktig funktion än den modell som representerar en rimlig uppskattning.

Tillgängliga data och beskrivningar har sammanställts för att kunna användas i den hydrogeologiska modelleringen av Aberg, Beberg och Ceberg. Tolkningen av data ger utrymme för olika alternativa uppsättningar av data (varianter) att använda i den fortsatta modelleringen. Den underliggande konceptuella modellen av berget är att det sätts samman av en bergmassa, som kan beskrivas som ett rumsligt varierande stokastiskt kontinuum, genomkorsat av mer vattengenomsläppliga sprickzoner, som också beskrivs som stokastiska kontinua men med andra egenskaper än bergmassan. Vidare delas modellen upp i en regional modell och en platsskalemodell innesluten i regionalmodellen. Platsskalemodellen beskriver bergmassan som ett stokastiskt kontinuum och beskriver de mer ledande strukturerna relativt detaljerat. Regionalmodellen innehåller färre detaljer och beskriver bergmassan med konstanta ekvivalenta hydrauliska parametrar. Dessutom används diskreta nätverksmodeller och kanalnätverksmodeller i fåtal fall som alternativa modeller i platsskalan.

I det följande beskrivs hur olika resultat från grundvattenflödesmodelleringen används vid modelleringen av radionuklidfrigörelse och transport i närområdet, fjärrområdet och biosfären.

Flödesrelaterade transportparametrar - närområde

Närområdesmodellen COMP23 beräknar icke-stationär transport av radionuklider i närområdet av ett förvar. Nuklider som frigörs från bränslet och lämnar kapseln diffunderar genom bufferten och transporteras vidare längs olika vägar till det strömmande grundvattnet i bergets sprickor. Den primära flödesrelaterade parametern här är grundvattenflödet (darcyhastigheten) i kapselskala. Denna information erhålls från analyserna med den stokastiska kontinuummodellen i platsskala, kompletterad med resultat från den diskreta nätverksmodellen. Den rimliga uppskattningen väljs som medianen av basfallet för respektive plats, medan det pessimistiska fallet väljs som 95%-tilen av den variant som har de högsta darcyhastigheterna för respektive plats. Man bör dock uppmärksamma att skillnaden mellan varianter (för samma plats) är relativt liten. Den mesta spridningen härrör från den rumsliga variationen inom en realisering.

Flödesrelaterade transportparametrar - fjärrområdet

Fjärrområdestransport modelleras med en strömtubsansats, där ”transporttider” och läge av utströmningsområde för ett antal endimensionella strömtuber erhålls från s.k.”partikelspårning” i den hydrogeologiska platsskalemodellen. Den endimensionella transportmodellen, FARF31, hanterar advektion och dispersion längs strömningsvägen, matrisdiffusion kombinerat med sorption på bergmatrisen samt radioaktivt kedjesönderfall. Fördröjningen i berget (”retentionen”) beror i mycket hög utsträckning på det s.k. ”transportmotståndet”. Detta kan uttryckas som kvoten mellan den flödesvätta ytan per volym berg gånger transportvägens längs och darcyhastigheten, eller med andra parametrar, som produkten mellan vattnets ”transittid” och flödesvätta ytan per volym vatten i transportvägen.

Resultaten av grundvattensimuleringar i platsskala med den stokastiska kontinuumsmodellen utgör den huvudsakliga informationskällan för de flödesrelaterade transportparametrarna. Skattningar av den flödesvätta ytan per volym berg erhålls dock från utvärdering av ett fåtal platsspecifika spårförsök, geologisk karakterisering, hydrauliska test och modellering. I huvudsak bestäms det skattade värdet av den flödesvätta ytan från skattningar av den konduktiva sprickfrekvensen, som i sin tur skattas från de hydrauliska testerna. Ett flertal antaganden behöver göras för att kunna hantera bristen på adekvata data för en del av de ingående parametrarna. Transittiden som motsvarar ”rimlig uppskattning” väljs från medianen hos basfallet av den stokastiska kontinuummodellens resultat, medan den pessimistiska transittiden väljs som 95%-tilen av den variant som har de kortaste transittiderna. Dessutom väljs pessimistiska värden av den flödesvätta ytan en faktor 10 lägre än värdet som motsvarar rimlig uppskattning. Det kontrolleras att kombinationen av transittid och flödesvätt yta tillsammans representerar avsedda ”transportmotstånd”.

Biosfär

Biosfärsmodelleringen syftar till att beskriva omsättningen av eventuellt utsläppta radionuklider i biosfären for att kunna göra det möjligt att uppskatta radiologiska konsekvenser för potentiellt exponerade grupper (människor) och för miljön. Varje plats delas först in i *typmoduler* för olika ekosystem och för varje typmodul beräknas *ekosystemspecifika dosomvandlingsfaktorer* (EDF). De moduler som nu används är *brunn, sjö, rinnande vatten, kust (hav), jordbruksmark och torv.* I den slutgiltiga analysen beräknas doskonsekvenser (Sv/år) med modellen BIO42, som multiplicerar utsläppet från geosfären (i termer av Bq/år) med de EDF-värden (Sv/Bq) som gäller för den modul i vilket utsläppet sker.

Känslighetsanalyser antyder att osäkerheten i EDF för en given modul typiskt är cirka två storleksordningar. Valet av modul har dock större betydelse – skillnaden mellan en modul med stor utspädning (öppen kust) och en med liten utspädning (brunn eller torvmosse) uppgår till många storleksordningar. Den rimliga uppskattningen är att välja den modul som anges som utströmningsområde för utsläppet i den hydrogeologiska modelleringen. Den pessimistiska uppskattningen är att välja den modul som ger den högsta dosraten (dvs. vanligen brunn, torv eller jordbruksmark).

1 Introduction

1.1 Background

This report concerns integration of data and data uncertainties in the radionuclide transport calculations evaluated within the SR 97 safety assessment project (/SKB, 1999a). SR 97 explores hypothetical repositories at three different sites; Aberg, Beberg and Ceberg with data taken from Äspö, Finnsjön and Gideå, respectively. From here onwards, this report will refer to the different sites as Aberg, Beberg and Ceberg.

The model chain for radionuclide release and transport calculations is made up of series of coupled models, which in turn require input from analyses of the state of the barriers and the rock. Each such specific evaluation also evaluates the uncertainties in the data delivered. The current report aims at integrating this information by trying to push the uncertainty discussion to a similar depth for the different underlying analyses, to explore potential correlations between uncertainties by tracking sources for uncertainty, and suggests input data for the analysis.

1.2 Objectives and scope

The objectives of the work undertaken is:

- to establish a framework for handling data uncertainty within SR 97,
- to complete the uncertainty discussion from the different underlying analyses which provide input to the model chain,
- to suggest and motivate ”reasonable” estimates, and ”pessimistic” estimates,
- to suggest ”probabilistic distributions” for the parameters where such distributions can be motivated.

The evaluation only concerns the potential impact of the repository for spent nuclear fuel (SFL-2).

The uncertainty evaluation focuses on data uncertainty for the scenario assuming some initially defect canisters. Evidently, quantitative release and transport calculations are only of interest in scenarios where canisters in fact fail. Scenarios, which do not assume or lead to defect canisters, or uncertainties in such scenarios, are not addressed here. The uncertainly evaluation also concentrates on the quantitative models and analyses selected for the model chain. The issue of conceptual model uncertainty is partly included in this evaluation. However, the more fundamental questions concerning model selection and which potential model couplings to analyse are not addressed here.

These latter questions are addressed in the SR 97 “Process report” /SKB, 1999b/), an underlying report to SR 97, or directly in the main SR 97 report /SKB, 1999a/. (The following text will from here on refer to these documents as the SR 97 Main Report and the SR 97 Process Report, respectively).

1.3 Organisation of report

The report is organised as follows. Chapter 2 generally discusses uncertainty and the concepts of reasonable, pessimistic and probabilistic estimates. The chapter thus provides the framework for the analysis in the report. Chapter 3 briefly presents the definition of the initially defect canister scenario and the main components of the model chain to be used for analysing this scenario. Chapters 4 to 8 discuss the uncertainty in the different analyses of the model chain and suggests reasonable and pessimistic parameter values. Chapter 9 concludes the report.

2 Framework for handling data uncertainty in SR 97

This chapter discusses the framework for handling data uncertainty in the model chain for radionuclide transport calculations and in the supporting analyses producing input data to these calculations. The concepts of ”reasonable”, ” pessimistic” and ”probabilistic” estimates are also given practical definitions for use within the project.

2.1 Uncertainty concepts

In general, uncertainty can be described as a lack of knowledge. Uncertainties are often categorised in order to better understand the origin of the uncertainty. Spatial variability is not uncertainty, but is related to uncertainty. These differences needs to be understood and properly handled when modelling geologic media, which usually are very heterogeneous. In order to evaluate the impact of uncertainty it is necessary to quantify the uncertainty.

2.1.1 Uncertainty categories

Traditionally, see e.g. NEA (1991), uncertainty in performance assessment is divided into *scenario uncertainty*, *conceptual model uncertainty* and *data uncertainty*. The exact meaning of these categories vary slightly between different performance assessments (NEA, 1997). Here the following concepts are used:

- Scenario uncertainty concerns uncertainty in the repository evolution caused by initial (uncertain) internal conditions or by future (uncertain) external conditions for the repository system analysed.

- Conceptual model uncertainty concerns uncertainty in the modelling of a process or uncertainty in the character of the geometric structure when modelling a process. On a general level this also concerns which processes (thermal, hydrological, mechanical or chemical) as well as couplings between these processes that need to be modelled in the assessment.

- Data uncertainty concerns uncertainty in the parameter values of a specific model.

These definitions also agree fairly well with the definitions suggested in the NEA (1997) document.

As already mentioned in the introduction, this report deals solely with data uncertainty and aspects of conceptual model uncertainty for the quantitative models and analyses of direct use in radionuclide transport calculations of the initially defect canister scenario. The other uncertainty issues are handled in other reports (mainly in the SR 97 Process Report and in the main SR 97 report).

2.1.2 Spatial variability

Many properties, geological in particular, exhibit *spatial variability.* The spatial variability of a property may itself be uncertain. In addition, spatial variability alone may amplify consequences of other uncertainties.

Uncertainty in spatial variability is usually handled by the concept of a stochastic process, which concern uncertainty in a function rather than in a single value. It will generally be harder to predict the value of a strongly spatially varying property, than from a smoother one, since knowledge of the property at one point, which could be obtained from measurements, provide less knowledge of the value of the property in adjacent points.

Spatial variability may propagate and amplify consequences of other uncertainties, also when there is no uncertainty in the spatial variability. For example, consider the consequence of canister failure in a repository. As will be discussed later in the report, the location of a single failed canister is probably completely random, but the consequence of the failure in terms of release and subsequent migration through the rock will depend on the canister location since the rock properties vary strongly in space. This means that if a single canister fails, but the location of the failure is uncertain, the uncertainty of the resulting release would reflect the spatial variability of the different release paths. It should be noted that this uncertainty would not decrease even if there was perfect knowledge of the spatial variability of different release paths, since the point of release is unknown.

The uncertainty created by spatial variability depends on the scale of the problem. If many canisters were to fail (at the same time) the full range of migration paths will actually be ”used” and spatial variability would cause temporal and spatial spread of the release rather than amplifying the uncertainty. (One could alternatively say that if many canisters fail, the failure location uncertainty decreases).

In summary, understanding spatial variability is essential when assessing geologic repository performance. The difference between variability and uncertainty has to be properly understood. The net effect on the uncertainty of the consequence depends on the specific situation being analysed.

2.1.3 Quantifying uncertainty and use of subjective information

Uncertainty in general implies lack of knowledge, but it is often possible to bound. If the analysed system performs well within the bounds of uncertainty, there is no reason to change the system or to seek more information in order to decrease uncertainty. Consequently, the means of quantifying uncertainty is crucial to the outcome, but also crucial for credibility of the performance assessment.

Probability distribution

The uncertainty of a single parameter can be expressed with a *probability distribution* or a *probability density function.* Depending on the nature of uncertainty, the form of the associated probability distribution can be discrete or continuous or a combination of both.

Probability distributions represent the main tool by which uncertainty can be quantified. However, when dealing with predictions of future behaviour or geologic properties between measuring points, traditional statistical estimates, based on repetitive experiments, are often not available or of limited validity. This may not necessarily mean that there is a complete lack of possibility to quantify the uncertainty. For example, it may still be possible to bound the parameters within an *interval* or to subjectively use expert opinion when judging the appropriateness of different possibilities. Such *subjective assessments* are opinions and judgements, based on experience and/or knowledge in a specific area, which are consistent with available information.

Clearly, there is a need for caution when using subjective probability information and as a rule of thumb the assessment results must not be critically dependent on the selected functional form of the density function. However, it should also be pointed out that failing to make any assessment of uncertainty, by just referring to lack of data for a full estimation of a density function is inappropriate for the performance assessment application. Without any uncertainty estimate the quality of the performance assessment results cannot be judged at all. In many cases the weak, but still defensible, form of uncertainty estimates, e.g. intervals, are sufficient to clearly demonstrate sufficient performance of the system studied. The range between reasonable and pessimistic parameter values may of course be seen as such an interval, but at occasions there may be more specific information on the distribution.

Correlation

The probability of an event may be affected by the outcome of other events. Such statistical dependence is extremely important to capture when assessing the probability of a series of events (e.g. a specific set-up of parameter values for an assessment code). For example, consider three events all with a probability of 10^{-2}. If these events occur independently the probability of all events occurring would be 10^{-6}, but if the events are fully correlated the probability for the joint event would still be 10^{-2}, i.e. a factor of 10^{4} higher.

Consequently, estimation of correlation between different parameters are extremely important to capture and it needs to be considered when formulating integrated calculation cases.

Stochastic process

In geologic media uncertainty often is not confined to a single value but rather concerns a function in space (and time). The function could be continuous, such as a temperature field or discrete, such as the distribution of fractures and fracture zones. Uncertainty in a function could be described by the concept of a *stochastic process*. Different possible outcomes of the function are called *realisations*. This means that the variability within a single realisation represents a suggestion for the spatial (or temporal) variability of the described property, whereas the spread between different realisations represents the uncertainty in the spatial (or temporal) variability.

2.2 Selection of input parameter values to explore uncertainty

According to the objectives of the present work the uncertainty evaluation should result in a reasonable and in a pessimistic set of input parameters, and also probabilistic distributions for the input parameters where there exists information that really can support the distributions selected. These concepts are further discussed below.

2.2.1 ”Reasonable” estimates

In accordance with the objectives the uncertainty evaluation should present ”*reasonable*” estimates of the parameters for the consequence calculations. The intention of presenting ”*reasonable*” estimates is to obtain a view on how the repository system would operate without making overly optimistic or pessimistic assumptions. Consequently, it seems natural to assume a unit probability of the *reasonable* estimates when the consequences of the case are compared with the regulatory risk limit of 10^{-6} (SSI FS 1998:1). However, it should be recognised that the likelihood of any exact outcome is zero and that the term ”reasonable” does not have a clear statistical meaning. The reasonable case is selected for illustration. Other cases need to be explored and evaluated against the regulatory risk limit. This is in accordance with the regulation, which requires an assessment of the uncertainties.

A ”reasonable value” must not necessarily coincide with a statistical mean or median. In general, neither of these values could be said to represent the most likely outcome. Furthermore, these statistical measures only have clear meanings for a given conceptual model, but in reality the selection between a ”realistic” analysis and a ”pessimistic” one usually concern the potential inclusion of uncertain processes in the analysis. Instead the pragmatic approach adopted here is that a reasonable value should be based on a model or direct measurements which are:

- plausible building on the present understanding of the phenomenon, where processes known, or generally thought, to be involved 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.

If simplifications are made they should still rather err on the pessimistic side, but no credit should be taken from the ”conservatisms” involved in the model.

The ”definition” is still judgmental and it should be evident that a ”reasonable estimate” may not be uniquely defined. Additional calculation cases are needed, which explore the range of uncertainty.

2.2.2 “Pessimistic” estimates

One way of bounding the impact of uncertainty is to construct ”*pessimistic*” estimates. A *pessimistic* estimate would mean selecting a parameter value (and conceptual model) within the uncertainty range, which maximises the consequence.

The main advantage of a *pessimistic* assumption is that it makes it possible to avoid a detailed description or analysis of a phenomenon which may be potentially beneficial, but would be very hard, or even impossible, to prove. It is thus primarily a means of handling conceptual model uncertainty. Omitting the description of such phenomena with a *pessimistic* assumption regarding its relevance would thereby increase the credibility of the safety statements. However, there are some major difficulties in making *pessimistic* assumptions:

- It is not always trivial to judge whether a statement/parameter indeed is *pessimistic* if several processes, e.g. if non-monotonous relations are involved, or simply because the knowledge of the phenomenon is too limited.

- Combining all pessimistic estimates into a “full” *pessimistic* case would be totally unrealistic and would grossly overestimate consequences as the combination of parameters making up the case will never happen in reality. Such as case should not be analysed since it would provide misleading guidance on the safety functions of different parts of the repository.

In light of the listed advantages and disadvantages with *pessimistic* estimates the following approach is adopted:

- The supporting analyses should concentrate on describing and quantifying uncertainties and correlation; *pessimistic* parameters for the integrated analysis level are based on an assessment of the uncertainties and correlations in the supporting analyses.

- *Pessimistic* assumptions made in order to simplify a supporting analysis can of course be made, but the conservatism has to be properly motivated.

Even if at one hand pessimistic values are unlikely, it is impossible to guarantee that none of the parameters in the calculations would take the pessimistic values.

Philosophically, there should always be room for the totally unexpected. There is also a judgemental aspect in the selection of pessimistic values.

2.2.3 Probabilistic estimates

Basing the performance assessment only on “reasonable” and “*pessimistic*” estimates may give quite misleading results regarding the actual performance of the repository. In particular, this is true if the results of the reasonable analysis and the pessimistic analysis deviate to a high degree. As already mentioned, the reasonable estimates are judgmental and even if they may represent the most plausible conditions there may be many other, and strongly deviating, conditions that are almost as plausible. The pessimistic estimates may, in contrast, overestimate consequences.

These problems could ideally be handled by analysing the probability distributions of the performance parameters, which then could be used to estimate a probability distribution of the radiological consequences. There are, however, several difficulties involved in estimating probabilistic distributions:

- usually there is little or no knowledge of the probability density function of the stochastic parameters, at most it is possible to identify intervals,
- there is often a need to discuss several stochastic variants resulting from e.g. uncertainty in stochastic parameters or different underlying conceptual models, but it is usually difficult to substantiate the degree of likelihood of different variants,
- in many instances different conceptual models or different stochastic parameters result in quite similar final results.

Given these difficulties the approach adopted in this report is to discuss the potential correlation between different parameters, but only suggest probabilistic estimates for parameters where there exist data or any other well founded means of motivating the distributions. Later, in the safety assessment, it may be motivated to use more “subjective” probability estimates when constructing probabilistic estimates, also for parameters without a well based support for such estimates. Such a discussion is conducted in the main SR 97 report, but lies outside the scope of the present report.

3 Input data and information flow in the model chain

The SR 97 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 and the rock. This chapter briefly outlines the main components and the information flow in this chain of models. Subsequent chapters will then evaluate the uncertainties in the information provided from the different analyses leading up the final consequence analysis.

3.1 Scenarios analysed

The scenario analysis of SR 97 is provided in the main SR 97 report. Some results of this analysis have implications for the work discussed in this report and are thus provided here.

The *base scenario* in SR 97 assumes the following conditions:

- All canisters are manufactured and sealed without defects. The repository is constructed according to specifications.
- Present day climate will prevail also in the future.
- Present day site specific groundwater chemistry and groundwater flow are assumed to be valid also in the future. Effects of landrise and other transients clearly observable today may still be considered.
- Rock mechanical conditions, including the stress field, will remain as they are today although the repository induced effects on creep, thermal expansion/contractions etc. are to be considered. However, future seismic events or changes to the mechanical boundary conditions are not considered.
- The conditions of present day site specific biosphere's will prevail also in the future. Effects of landrise and other transients clearly observable today may still be considered.

The evaluation of the base scenario, which will be covered in the main SR 97 report and in supporting documents, particularly concern evaluation of the canister life time. It can be expected that this analysis will lead to very long canister life times.

As post-closure radiological consequences only can occur in case canisters break and release radionuclides, the base scenario may not result in any consequences for an extremely long period of time. In order to explore the function of the other barriers of the repository system SR 97 also considers a scenario postulating some *initially defect canisters*. In addition, the scenario is also relevant since such initial defects may not be totally avoided. The initially defect canister scenario builds upon the following assumptions:

- All conditions, except those concerning the initial state of the canisters, are as for the base scenario.
- Some canisters are initially defect, the type of defects and their frequency are based on analysis.

Apart from these two scenarios, SR 97 evaluates other scenarios like changing climate scenarios and seismic scenarios. The present report cannot be used directly for all parameter input to these latter scenarios, but is of course useful for parameters not affected by the scenarios and also as a baseline for discussing values of parameters potentially altered by these scenarios.

3.2 The chain of models

The primary model used for evaluating radionuclide transport is made up of a series of coupled (sub-)models, which in turn require input from analyses of the state of the barriers and the rock as illustrated in figure 3.1.

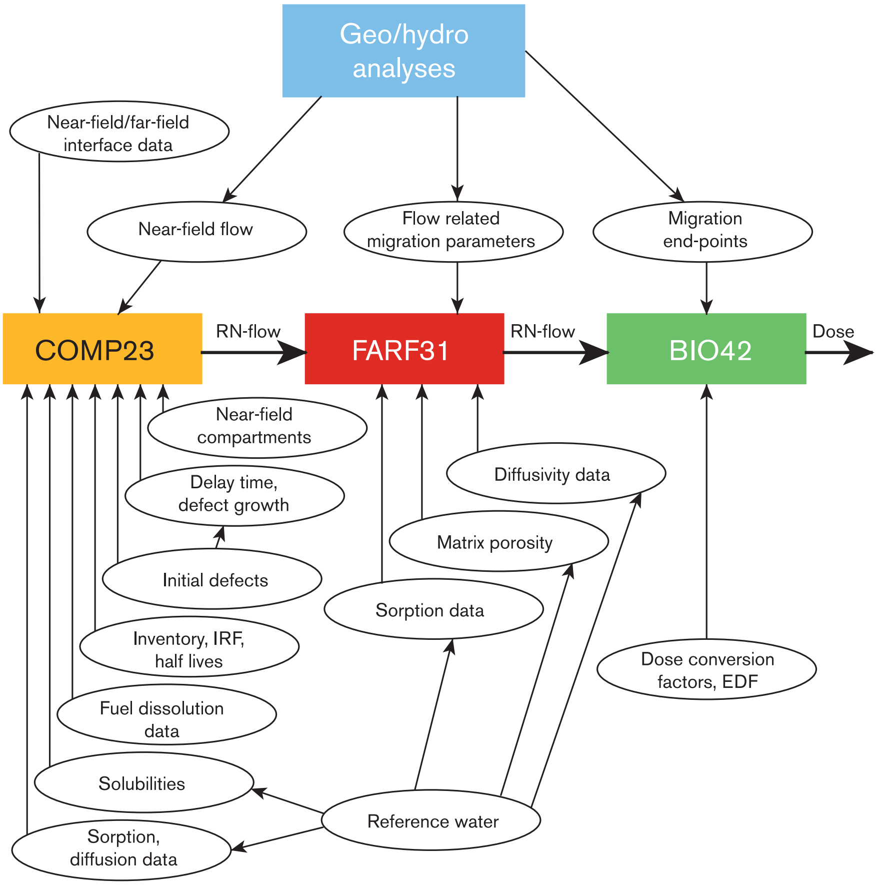


***Figure 3.1**. The chain of models used for evaluating radionuclide transport and the prime sources of information for these models.*

The direct radiological consequence analyses are performed by the near-field source term model COMP23 (Moreno and Gylling., 1998), the far-field migration code FARF31 (Norman and Kjellbert, 1990) and the code BIO42 (SKB, 1995) which transforms radionuclide flow into dose using pre-calculated ”dose conversion factors”. The various sources of information to these codes, also displayed in the figure, could in turn build on elaborate modelling combined with data analysis. For example, the hydrogeological input, schematically shown in figure 3.1, can be broken up into a hydrogeological chain of analyses as displayed in figure 3.2. It should be evident from both figures that evaluation of uncertainties of the radionuclide consequence analysis requires evaluation of the uncertainties in the different input sources.

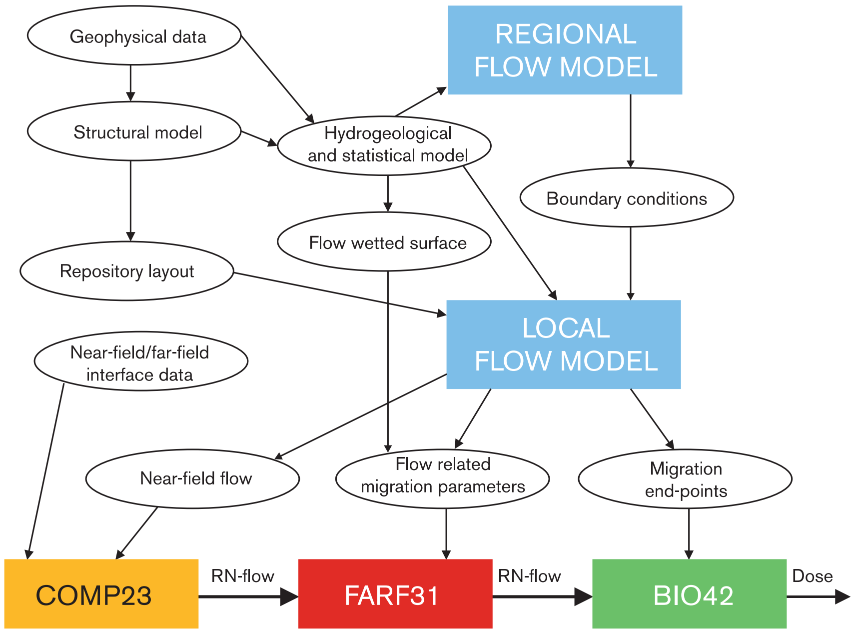


***Figure 3.2**: The different hydrogeologic analyses adopted used to provide the hydrogeologic input to the main chain of consequence codes*

More details of the different sources of information to the consequence codes will be provided in subsequent chapters, when discussing the uncertainty in the information delivered.

3.3 Probabilistic analyses - PROPER and Monitor 2000

A control program called PROPER administers execution of the chain of sub-models described in the previous section. The PROPER program (PROPER, 1996; PROPER MONITOR User’s Manual) allows both single executions of the model chain and probabilistic calculations.

In the latter case, a selection of the input parameters is given as distributions rather than as fixed values. The distributions are chosen so as to express uncertainties in the input parameters. The probabilistic calculations consist of many executions or realisations of the model chain. In each of these, a new set of values of the input parameters is sampled from the input distributions. Each realisation results in e.g. a curve, describing dose to man as a function of time. The ensemble of results from the different realisations can then be post processed to provide a statistical distribution of e.g. the maximum dose over time. In this way uncertainties in input parameters are reflected in the resulting distributions.

The PROPER program is equipped to perform traditional probabilistic calculations and post processing. Advanced statistical post processing and result presentation is carried out with the commercially available tools like STATISTICA and MATLAB. Input to the sub-models and to the PROPER control program is handled via the recently developed graphic user interface Monitor 2000 (Monitor-2000 User's Guide, 1998).

4 Spent fuel and canister data

4.1 Inventory

4.1.1 Source of data

Håkansson (1998) calculates inventories for two different burn-ups (38 MWd/kg U and 55 MWd/kg U) of BWR fuel elements (type SVEA with 96 rods) and for two different burn-ups (42 MWd/kg U, 60 MWd/kg U) of PWR fuel elements. Results are presented as activity in terms of actinides, fission products and activation products (in the metal parts) per tonne U. Uncertainties in these estimates are also discussed.

The calculations are mainly done using the ORNL SCALE 4.3 package (based on ORIGEN) (ORNL, 1996). For comparison calculations have also been conducted with the CASMO-4 code (Edenius *et al.*, 1993). Neutron cross sections, gamma cross sections and decay constants are taken from data bases in the SCALE package.

4.1.2 Use in SR 97, modelling approach and conceptual model uncertainties

The total inventories, for the fuel pellets and the metal parts, of the spent fuel in a canister are directly used as input in the near-field code COMP23 (Romero, 1995). In order to use the calculated inventories it is then necessary to make assumptions of which type of fuel and how much fuel are to be disposed in each canister. The fuel composition is constrained by the heat load and the space available in the canister.

The inventory calculations is made in steps where the first step is to calculate the burn-up of the fuel assemblies in order to find the isotopical composition at the time of discharge of fuel from the reactor. Inventories at later times are evaluated by considering radioactive decay. ORIGEN-S calculates nuclide content, activity and decay power.

The results depend on accurate calculation of self shielded exposure dependent cross section, which is specific to the reactor type and reactor conditions for the fuel during burning. The assembly code CASMO was used for comparison and neutronic verification of the actinide content.

Calculations are made only for the PWR and SVEA-96 BWR fuel. The small amount of mixed-oxide fuel now stored in CLAB has not been considered in the inventory estimates.

Calculations are performed for fuel burnt under average conditions to an average burn-up. In reality there will be an axially dependent burn-up where the highest exposure will be about 20% higher than the average. For individual fuel pellets this implies that the inventories may differ substantially due to differences in irradiation history. It is assumed, however, that much of this local variability is averaged out over a fuel element which consists of more than a thousand pellets.

Differences in burn-up between different fuel elements, as well as the difference between BWR and PWR fuel is also to a great extent evened out on the canister level, as the canister load is controlled by the heat load. In SKB 91 (SKB, 1992) a reference assembly of 8 BWR fuel elements were selected for a reference canister giving rise to a heat load of 950 W at the time of disposal. It was also shown that it is possible to combine fuel elements with different burn-ups and still reach an initial heat load around 1050 W. The canister and heat constraints used in SR 97 (Bäckblom, 1996) allow for more fuel elements per canister, but the technique applied should be the same (i.e. to make sure that the fuel element composition in a canister would still result in the same initial heat load).

4.1.3 Data uncertainties, correlations and dependencies on other parameters

The inventories are not affected by any other process considered in the calculation chain. According to Håkansson (1998) uncertainties arise primarily from uncertainties in the calculation models themselves but also for uncertainties in initial fuel composition, burn-up history and procedures for canister composition. Under the assumptions made, the main uncertainties are associated with the input data used in the calculations. The pure numerical errors involved in the analyses are small.

The calculations depend on three types of data:

- cross sections,
- yields,
- decay constants.

The decay constants are the most accurate of these data. The accuracy of half-lives of all important isotopes are 0.1% or better. The yields are measured and libraries are then constructed for least square fits for each isotope. This may lead to individual variations, but is considered accurate on the average. The cross section uncertainty is more complex.

The basic cross section data are measured cross sections and resonance parameters. For stable and long-lived isotopes the cross sections are well known for all reactor materials, but the uncertainties are larger for the short-lived isotopes. The significance of this uncertainty depends partly on the time frame for which the inventory needs to be calculated. The long term time scale (>100 years) is the primary focus of repository performance assessment. For this time scale the actinides are responsible for the main part of the activity, but are also very important for the fission products as the yield at least for the lighter fission product isotope depends on the fissioning nuclei.

Håkansson (1998) partly studies the impact of the cross-section uncertainty by comparing results from SCALE and CASMO. He concludes that the total uncertainty in actinides may be 20% and the total uncertainty in fission products may be 12%.

4.1.4 Quantification of uncertainties

It is suggested that the *reasonable* inventory should be based on the inventory calculated by Håkansson (1998) for 12 BWR fuel elements with a burn-up of 38 MWd/ kg U (Table 9 in Håkansson, 1998 and Table A.1.1.2 in appendix A). This is the most common canister assembly within the repository concepts studied. Clearly, about 25% of the spent fuel will originate from PWR, but mixed canister assemblies will not be considered. Instead it is suggested to qualitatively discuss the implications of PWR canisters (see next paragraph). It should be noted that this inventory estimate also *includes* activation products in the metal parts.

The uncertainties are mainly connected to uncertainties in burn-up and calculation method. Due to the chain-reactions inventories of different nuclides are also strongly interrelated. Consequently it is not appropriate to produce ranges of the uncertainty in the inventory of a specific nuclide. There is no evident motivation for forming a pessimistic case. On the other hand an uncertainty of 20% is almost negligible in comparison to other uncertainties in the calculation chain. Furthermore, preliminary assessment calculations suggest that variation of inventory has a negligible effect on release calculations as transport is limited by physical and chemical conditions in the repository. This means that it is permissible to discuss impact of inventory uncertainties in a qualitative manner and not to progress these uncertainties further down the calculation chain. Qualitatively the impact of the following should be discussed:

- effect of PWR fuel element canisters,
- effect of higher burn-up, while still maintaining the initial heat-load of the *reasonable* fuel composition,
- effect of the 20% actinide and 12% fission product uncertainty suggested by Håkansson (1998).

Given the lack of information and given the high chance that variability in the fuel pellet level will be evened out already at the fuel element level there does not seem to be a need to address spatial (i.e. from canister to canister) variability in inventory. However, in future assessments it may be worthwhile to also include the inventory of the MOX-fuel in the analysis.

Table 4.1 summarises the suggested quantification of inventory uncertainty.

Table 4.1: **Suggested quantification of uncertainty in inventory**

Case	Description
Reasonable estimate	Inventory estimated by Håkansson (1998) for 12 BWR 38 MWD/kg U after 40 years (i.e. table 9 in Håkansson (1998) and table A.1.1.2.
Pessimistic case	Not applicable.
Uncertainties	Qualitative evaluation of the impact on release from COMP23 due to i) effect of PWR canisters ii) effect of higher burn-up composition iii) uncertainty suggested by Håkansson (1998) while still keeping the initial heat load constant

4.2 Radionuclide release from the spent fuel

4.2.1 General

Use in SR 97

The source term heavily depends on the dissolution of the radionuclides in the spent fuel. The dissolution models used in the near-field model COMP23 (Romero, 1995) includes the following mechanisms:

1. immediate dissolution of a certain fraction of the inventory specified for each nuclide (IRF or instant release fraction),

2. release of the radionuclides contained in the UO_2 matrix at a rate R equal to the rate of the dissolution/conversion of the uranium dioxide matrix.

The modelling and data support for these mechanisms are obtained from different sources and are thus discussed separately in the section below.

4.2.2 Dissolution/conversion of the UO_2 matrix

Source of information

Different models for dissolution/conversion of the UO_2 matrix are discussed in SKB (1999). Input data is partially obtained from experimental data, but the final conversion rates to be used are based on various assumptions and modelling.

Modelling approach and conceptual model uncertainties

The largest amount of the radionuclides in the spent fuel is embedded in the UO_2 matrix and is thus contained there until the matrix itself dissolves. The release is a function of the UO_2 transformation. The dissolution/transformation of the UO_2 matrix is mainly controlled by redox conditions (see e.g. SR 95, SKB, 1995 or SKB 91, SKB, 1992).

Experiments carried out under oxidising conditions (SKBF, 1983, p. 11.4) show that the dissolution rate then is less than 10^{-4} yr^{-1}. In the repository, the dissolution rate will be much less since the water chemistry there is much more favourable.

In deep natural groundwaters and in groundwater in contact with the engineered barriers pH and redox conditions are such that UO_2 is thermodynamically stable and the release would be controlled by the solubility limit of UO_2. This model may, however, underestimate the fuel conversion rate since radiolysis where the α-dose rate of the fuel disintegrates the water may lead to production of oxidants. Still in process report SKB (1999) it is noted that the abundance of iron inside the canister and the comparatively low dose rates in question makes it possible that only little oxidation in fact would occur. This conclusion can also find support from anoxic leaching experiments with spent fuel.

Radiolysis disintegrates the water into equal parts of oxidising and reducing species, but one of the reducing species, H_2, reacts much more slowly than the oxidising species, which under certain conditions could result in a net-oxidation of the fuel. A radiolytic dissolution model depending on the α-decay rate was first suggested by Werme *et al.* (1990) and has since been applied in many assessments, including SKB 91 (SKB, 1991), SKI Project-90 (SKI, 1991), TVO-92 (Vieno *et al.*, 1992) and SITE-94 (SKI, 1996). However, it is suggested that this model strongly overestimates the dissolution. For SR 97 (Eriksen, 1996 and Eriksen, 1999) a more developed model has been developed with the following features:

- the reactions occur in a thin water layer (100μm) between the fuel pellets and the (defect) cladding,
- both α and β radiolysis is considered,
- the reactions between the oxidants H_2O_2, O_2 and the uraniumdioxide is considered to be first order reactions (i.e. the rate is proportional to the oxidant concentration) and the reaction rates are taken from experimental measurements,

- the H_2 created will not leave the system, which can be motivated by the larger partial pressure of H_2 created by corrosion of the iron inside the canister,
- around 40 reactions are considered.

The assumption of the reactions to be first order could certainly be questioned even if a first order reaction appear to be the reasonable assumption (SKB, 1999a). There are measurements, which may imply a lower order (square root) dependence between rate and oxidant concentration. If this is the case the extrapolation towards low oxidant concentration assuming first order reactions may result in a significant underestimation of the reaction rate. Unfortunately it is not possible to carry out reaction rate measurements at the low concentrations that may be relevant for the spent fuel conversion which means that the reaction rate dependence needs to be left as a conceptual model uncertainty.

Data uncertainties, correlations and dependencies on other parameters

Sensitivity analysis Eriksen (1996) and Eriksen (1999) with the new dissolution model suggest the following dependence of other parameters:

- the dose rate has little impact on the oxidation rate of the fuel, which means that the dissolution rate can be considered constant throughout the entire analysis,
- the water layer thickness (i.e. the gap between fuel and cladding) is uncertain, but calculations result in the same rates in the range 100 μm - 1000 μm (for 40 μm the rates decreases),
- the oxidation rate of the fuel appears to be directly proportional to the reaction rate of H_2O_2, whereas the reaction rate of O_2 is of minor importance,
- the initial content of H_2, which may originate from the steel corrosion, has very limited impact on the oxidation rate of the fuel for times longer than a year.

Simulation with reference values (a layer thickness of 100μm and a H_2O_2 reaction rate of $2.2 \cdot 10^{-10}$ dm/s) results in a dissolution rate $R=10^{-8}$ per year (Eriksen, 1996 and Eriksen, 1999). The layer thickness corresponds to the thickness of the gap at manufacturing, which is 100 μm, but could of course increase at later times. However as mentioned above, larger thickness have very little impact on the calculated rate.

Due to measurement technique limitations measurements of the H_2O_2 reaction rates have been confined to much higher oxidant concentrations than assumed in calculations and the extrapolation of the rate to lower concentrations could of course be questioned. Much lower rates would imply negligible radiolytic conversion (i.e. the UO_2 solubility model would be correct) and cannot be excluded. Much higher rates appear to be in conflict with indirect evidence such as the occurrence of U(IV) mineral in laboratory experiments, but cannot again be fully excluded.

Quantification of uncertainties

The refined fuel conversion model attempts at a realistic description of the fuel oxidation and resulting dissolution rate. This model, using the reference input assumptions leading to a dissolution rate of $R=10^{-8}$ yr^{-1} should consequently be taken as a *reasonable value*. However, it should be pointed out that the model still builds on some non-proven assumptions (see above), implying that other rates could in fact also be possible.

A lower value would be to conversion rate controlled by the solubility of the UO_2 matrix, but also higher conversion rates could not be excluded based on present day knowledge. It is not really possible to suggest a *pessimistic* fuel conversion rate. Clearly immediate dissolution of the fuel ("instant coffee") is a theoretical upper bound, but this "rate" is too extreme and unrealistic to be passed on as a meaningful pessimistic value. Instead it is suggested to only provide the reasonable value for calculations and then only discuss possible implications of the uncertainty of dissolution rate.

The different cases are summarised in table 4.2.1.

Table 4.2.1: Suggested quantification of uncertainties in fuel conversion

Case	Description
Reasonable estimate	Constant dissolution rate 10^{-8} yr^{-1}
Pessimistic case	Not meaningful – discuss implications of uncertainty in safety assessment

4.2.3 Instant Release Fraction (IRF)

Source of information

Johnsson and Tait (1997) evaluate the instant release fraction (IRF) for the different radionuclides in the spent fuel. They also discuss uncertainties. Their analysis builds on measurements of fission gas releases (FGR) from representative Swedish BWR fuel combined with information from leaching studies on LWR and CANDU fuel.

In addition, it is necessary to account for the activation products in the metal parts. The inventory of these nuclides is part of the total inventory estimate of Håkansson (1998), as already discussed in section 4.1. No special study of the release of activation products from the metal parts has been undertaken within the framework of SR 97. Instead the modelling is handled by pessimistic assumptions.

Modelling approach and conceptual model uncertainties

A small percentage of the inventory of a few radionuclides is located at the fuel-clad gap and at grain boundaries in the fuel. Experiments show that the fuel-gap fraction releases very rapidly upon contact with groundwater. The grain-boundary release is slower, but still much faster than the matrix dissolution. Also the activation products in the metal parts could be assumed to be released much more rapidly than the nuclides in the spent fuel itself.

In COMP23 it is assumed that both the fuel clad-gap fraction, the grain boundary fraction and the inventory in the metal parts immediately release to the groundwater, which is represented by a combined source term referred to as the Instant Release Fraction (IRF). This simplification is apparently pessimistic (it would overestimate the release), but probably only mildly so. Furthermore, the impact of the simplification on the release from the canister is probably very small given the delay time and the transport resistance in the bentonite.

Uncertainties, correlations and dependencies on other parameters

The IRF in the fuel itself is influenced principally by in-reactor irradiation conditions with a few exceptions. Redox conditions have a major impact on the IRF of ^{99}Tc (Forsyth and Werme, 1992) with anoxic conditions greatly reducing the release. For ^{14}C and ^{129}I the IRF increases significantly as the temperature is increased from 25 to 100 °C, whereas there is a slight increase with temperature for ^{137}Cs and ^{99}Tc. However, Johnson and Tait (1997) propose to use oxidising values for ^{99}Tc and high temperature values for the other nuclides, thus pessimistically de-coupling the observed dependencies. Given the initially high temperatures and locally likely oxidising conditions at the fuel pellets these simplifications seem highly warranted.

The derived IRF values are subject to different types of uncertainties,

- the assumption of a correlation between fission gas release (FGR) and IRF for certain nuclides,
- the method of determining the distribution of fission gas release in representing the full assembly of fuel elements and canisters,
- the radiochemical measurements,
- limited data or use of qualitative information from post-irradiation examination studies of spent fuel.

It is assumed that the IRF are directly proportional to the FGR for ^{137}Cs, ^{135}Cs, ^{129}I, ^{36}Cl. For some of these nuclides, notably ^{135}Cs and ^{137}Cs this relation finds strong support from measurements. In other cases pessimistic values are selected. For nuclides not dependent on FGR (^{99}Tc, ^{90}Sr, ^{14}C) estimates are based directly on radiochemical measurements mainly on CANDU fuel. Reasonable and extreme values are reported.

Estimates of FGR are based on measurements from a very large number of fuel rods and several studies on BWR fuel, with different burn-ups (20 - 45 MWd/kg U). This database appears to be extensive in order to judge variability and uncertainty in FGR. However, Johnson and Tait (1997) only reports on ”reasonable” ”average” FGR and ”pessimistic” ”average” FGR, and the question arises whether the observed spread in FGR should be considered as a spatial variability in a repository or if fuel rods with different FGR:s will be mixed when assembling the canisters. Given the fact that canisters will be assembled to a specific heat load (see section 4.1), it will be assumed that the ”average” values and the range provided by Johnson and Tait (1997) refer to canisters and concern uncertainty rather than spatial variability.

Johnson and Tait (1997) claim that uncertainties arising from radiochemical measurements are very small. The largest possible sources of error arise in the determination of ^{14}C, ^{36}Cl and ^{129}I releases. These uncertainties are considered when suggesting the pessimistic values of the IRF.

In some cases, the limited data raise questions about the uncertainty in the estimated IRF values. The significant database on release of ^{36}Cl, ^{14}C and ^{129}I from CANDU-fuel and the clear correlation with gas release suggest that the values are pessimistic. For some nuclides (e.g. ^{79}Se, ^{108m}Ag, ^{113m}Cd and ^{107}Pd) there are no data on release during leaching. These elements are likely to be in metallic form in the spent fuel and would therefore be expected to have very small IRF values. The uncertainties are large, however, and Johnsson and Tait suggest using the IRF values for ^{129}I and ^{137}Cs, which are considered to be more volatile during reactor irradiation. Johnson and Tait (1997) also present some experimental indication that the assumption on conservatism is correct.

Regarding the metal parts, evaluation of the inventories calculated by Håkansson (1998) shows that ^{94}Nb, ^{59}Ni and ^{61}Ni almost only occur in the metal parts. For simplicity IRF should be set to 100% for these nuclides even if there may be a limited dissolution rate of the steel. Regarding ^{14}C, Antilla (1992) suggest that the inventory is shared between the fuel (50%), the cladding (40%) and the metal parts (10%). Given the durability of the cladding it seems reasonable to only add another 10% IRF for ^{14}C as a reasonable value, but assume another 50% as a pessimistic value.

Quantification of uncertainties in SR 97 calculation cases

Based on the arguments provided in previous sections it appears evident that a reasonable *estimate* of the IRF for different nuclides are the values given by table 4.2.2. These values have been produced by combining the values of table 3 in Johnsson and Tait (1997) with the additional assumptions concerning the metal parts discussed above. Clearly, the reasonable values suggested by Johnsson and Tait (1997) rather seem to represent mean values in a distribution than a process based estimate. However, given the averaging connected to the assembly of fuel elements in canisters it appears reasonable to assume averages as a good representation of the canister inventory. The pessimistic assumptions included in the estimates also seem difficult to avoid without an extensive measurement programme on the actual spent fuel produced in the Swedish programme.

In a similar fashion it appears reasonable to select the pessimistic estimate column in table 4.2.2 as a *pessimistic* case.

Table 4.2.3 summarises the suggested quantification of uncertainties in IRF to explore in SR 97.

Table 4.2.2: *Reasonable and pessimistic IRF values for some key nuclides (taken from table 3 in Johnsson and Tait,* 1997*, combined with assumptions concerning the metal parts).*

Nuclide	***IRF(%) reasonable estimate - only fuel***	***IRF(%) reasonable estimate including metal parts***	***IRF(%) pessimistic estimate***
C-14	5	15	55
Cl-36	6	6	12
Co-60	-	-	-
Ni-59	-	100	100
Ni-63	-	100	100
Se-79	3	3	6
Kr-85	2	2	4
Sr-90	0.25	0.25	1
Zr-93	-	-	-
Nb-94	-	100	100
Tc-99	0.2	0.2	1
Pd-107	0.2	0.2	1
Ag-108m	3	3	6
Cd-113m	3	3	6
Sn-126	2	2	4
I-129	3	3	6
Cs-135	3	3	6
Cs-137	3	3	6
Sm-151	-	-	-
Eu-154	-	-	-
Ho-166m	-	-	-
Actinides	-	-	-

Table 4.2.3: *Suggested quantification of uncertainties in IRF*

Case	**Description**
Reasonable estimate	Use reasonable estimate (including metal parts) in table 4.2.2
Pessimistic case	Use pessimistic estimate in table 4.2.2

4.3 Canister defects and delay time

4.3.1 Introduction and application in the model chain of SR 97

According to Werme (1998) the canister will be designed such that it will fully isolate the waste and such that no known corrosion process would lead to a failure before 100 000 years. There it is also stated that these conditions are attainable for the canister design used for SR 97. Furthermore, the assumptions of the SR 97 *base scenario* are evaluated in the SR 97 assessment (SKB, 1999a). This will most likely lead to canister lifetimes considerably longer than 100 000 years, but this evaluation lies outside the scope of the current report.

The only possibility for canister failure under the base scenario conditions would be a development of initial defects not discovered in the quality control. Such defects cannot be fully excluded and are covered by the initially defect canister scenario. Initial defects leading to loss of isolation may in turn lead to radionuclide releases, the impact of which needs to be assessed quantitatively.

The assessment calculation in COMP23 (see chapter 3) needs to be supplied with the *frequency* of defects, the *size* of the defects and the *location* of the defect on the canister. The initial defect may *grow* with time due to the corrosion of the steel vessel. Furthermore, a continuous water path needs to be established between the fuel rods and the defect before radionuclides can migrate from the fuel out from the canister. In COMP23 the time it takes to establish this connection is handled by introducing a *delay time* before commencement of the release. Obviously, initial defects, defect growth and delay time are interrelated and are thus treated together in this section.

4.3.2 Initial canister defects

Source of information

At the current stage of development of the SKB Programme there does not exist an experience from an industrial scale manufacturing, loading, welding and quality control of canisters. Consequently, estimates on size and frequency of initial canister defects has to rely on a series of speculation. Building on an assessment of electron beam welding by Punshon (1997) the *author* of this report together with *SKB staff* instead provide reasoned arguments for potential sources for defects and how they may remain undiscovered. These reasoned arguments, together with the conclusions drawn are reported in the following.

Modelling approach and uncertainties

There is no real experimental database that can be used to estimate size and frequency of initial canister defects. Still, given the extremely good possibilities of inspection canisters before encapsulation it appears that the only realistic location of the defects would be in the weld of the lid. Punshon (1997) identifies several following potential causes for defects including that the beam misses the joint between canister and lid, insufficient depth of weld, porosity, cavities, root defects, surface defects, fractures and defects caused by flash-over in the electron cannon. Of these, only a beam missing the joint or flash-over in the electron beam could lead to an initially un-tight canister.

It appears very hard to conceive a case where a defect in the weld would not be discovered by ultra sound and from visual inspections of the welded canister. The defect has to be very thin (less than 1 μm) if it would not show up on ultra-sound. A defect affecting the whole circumference of the weld would easily be discovered when lifting the canister.

Quantification of uncertainties

Based on the reasoned arguments it appears that the most likely position of the defect would be at the weld of the lid. Considering the chance of discovering weld defects it also appears that the maximum initial defect height would not exceed 1μm. One may further assume that this defect extends at the most half a circumference, i.e. approximately 1m, since otherwise the defect would be discovered when lifting the canister. This results in a defect size of about 1 mm^2 located at the lid. It should also be noted that this position would minimise the length of the migration paths to a potential disturbed zone, implying that alternative positions of the defect (which indeed seem totally unlikely) can be also be pessimistically discarded. In addition, it should pessimistically be assumed that this position will also coincide with the position of the fractures (if any) intersecting the deposition hole, minimising the length of this direct migration path (see also section 7.2).

Building on the arguments presented it also appears that the chance of not discovering defects is close to zero. Consequently it could be argued that the reasonable value of the canister defects is a zero frequency. Still, it needs to be admitted that one may conceive internal defects of the weld (e.g. air bubbles), which would not be immediately possible to discover on the surface of the canister, even if an ultra-sound test may discover the defect. As a design criterion the canisters must be fabricated, sealed and inspected with methods that guarantee that no more than 0.1% of the finished canisters will contain defects that are larger than the acceptance specification for non-disturbing testing (Werme, 1998). The actual number of initially defect canisters will be less than 0.1%.

Given the very low defect frequency it is believed that the defects occur almost randomly, which means that there will be no correlation between the positions of canisters with defects. However, if the failure frequency had been higher a spatial correlation may be assumed, as such a high frequency probably would be caused by some (temporary) failure of the quality control of the filled canisters. In that, hypothetical, case it may be quite likely that all these canister would be disposed in the same tunnel given that these canisters could belong to the same batch.

Under the restrictions of the initial canister defect scenario it appears that the reasonable initial canister defect is to assume just a single initial defect canister with a 1 μm thin defect with a total area of 1 mm^2. A more pessimistic case would be to adopt the 0.1% defect ratio, but with the same initial defect size since (even) larger initial defects are considered most unlikely. Table 4.3.1 summarises these suggestions.

4.3.3 Growth of defect and delay time

Source of information

Bond *et al.* (1997) have analysed the growth of defects and the time delay before a continuous water path from the fuel elements out to the bentonite is created. An uncertainty evaluation of their analysis is made in SKB (1999) which also discusses copper corrosion and potential failures of initially intact containers. The work of Bond *et al.* is primarily based on modelling considerations.

Modelling approach and uncertainties

According to Bond *et al.* (1997) the defect grows when the corrosion product (magnetite) resulting from the corrosion of the steel vessel eventually will strain the copper vessel. If the corrosion is local around the defect, this will eventually lead to a disc-shaped burst (diameter around 1 dm) through the copper container for a more wide spread corrosion the failure would finally occur at the lid.

Radionuclides may migrate from the failed canister also when there is a small defect, but migration cannot start before there is a continuous path between the fuel rods and the defect. The time it takes for development of such a path is called the *delay time*. The delay time is controlled by the bentonite permeability, the size of the defect, but also by the development of a gas overpressure due to the corrosion, which will resist the water flow.

Bond *et al.* (1997) discuss the following factors which may affect these estimates:

- *Corrosion rate.* The failure time is roughly proportional to the corrosion rate. Higher rates than 0.1 µm/year are considered highly improbable over longer times.

- *Initial defect position.* One scenario is studied where the defect is located at the bottom of the container. In this case the initial (small) amount of water inside the canister is expelled from the canister when the internal pressure in the canister exceeds the external hydrostatic pressure. In this scenario a small amount of contaminated water is expelled in the time span of 0.8 - 1.5·10^4 years.

- *Initial size of defect.* For defects smaller than 8.25 mm^2 corrosion will be limited by the diffusion of water vapour. For much larger defects the critical question is whether also the steel container has a crack. If the steel container is intact the corrosion of the steel will still result in a penetration time of the order of 2·10^5 year, but if the steel contains a crack "*the time at which radionuclides are first released from the canister is short*"

- *Initial shape of defect.* The water inflow to the canister will be much faster for a thin, rather than a circular defect of the same area. For a 1 mm^2, but thin defect the inflow of water will be 200 times larger than for a circular defect, which means that it is unclear whether a gas over-pressure will have time to develop.

Clearly one critical factor is the steel corrosion rate. Bond *et al.* (1997) discuss the influence of temperature, salinity, pH, hydrogen overpressure and galvanic coupling on the rate. It is concluded that the influence of temperature and pH can be treated as independent in Swedish granitic groundwaters, but that the influence of salinity and hydrogen overpressure is not entirely clear. It is also suggested to explore a ten times lower corrosion rate (i.e. 0.01 µm/year). It is stated that there is no evidence to suggest that a rate higher than 0.1 µm/year will be sustained under likely repository conditions. It is stated that the largest uncertainty is associated with the extrapolation to very long periods of time.

In addition, at least the following uncertainties of the analysis need to be considered:

- The analysis does not consider the effect of thermal expansion combined with the bentonite swelling pressure. However, mechanical analyses of intact canisters (Cakmak, 1994) shows that there are no stress changes (and consequently no deformation) over the welded parts of the canister.

- When failure occurs, after very long times, this may affect the geometry and chemistry of the bentonite buffer. This impact has not been quantified in the present study.

Quantification

With a realistic estimate of the iron corrosion rate (0.1 µm/year) Bond et al. (1997) suggest that a large damage will not occur before $2 \cdot 10^5$ years and before this time the defect size is almost unchanged. For a very pessimistic estimate of the corrosion rate (1.0 µm/year) the damage will not occur before 22 000 years. These two failure times are used as *reasonable* and *pessimistic* estimates respectively.

Results of modelling water inflow combined with hydrogen formation due to corrosion for a 1 mm^2 circular defect suggest a delay time of $2 \cdot 10^5$ years. This time is taken as a *reasonable* estimate. However, one may pessimistically assume that the gas pressure inside the canister would not build up sufficiently fast to control the water inflow and that the defect has another shape. Accounting for uncertainties in bentonite hydraulic conductivity and in the shape of the defect would then imply a very *pessimistic delay time* of 300 years.

4.3.4 Quantification of uncertainties

The estimates of initial defect size and frequency (motivated by reasoned arguments partly building on Punchon (1997) as well as the estimate of the following failure growth by Bond *et al.* (1997) attempts at a realistic description of what will actually happen. Consequently these estimates, i.e. a single initial failure at the lid of a size of 1 mm^2 and a delay time of $2\cdot10^5$ years followed by a “complete damage”, i.e. a failure large enough not to offer any migration resistance, could be taken to represent a “*reasonable estimate*”.

As already argued in section 4.3.2 a *pessimistic assumption* on the initial failure would be 0.1 % of all canisters (i.e. 5) with an initial failure of 1 mm^2 at the lid. According to section 4.3.4 pessimistic estimates of the delay time is 300 years and a pessimistic estimate of the time to complete canister failure is 22 000 years.

Finally, one variant should explore the ”the water exclusion case” suggested in Bond *et al.* (1997) to make sure that it is insignificant to the continuous release cases.

The suggested cases are summarised in table 4.3.1

Table 4.3.1: *Suggested quantification of uncertainties in canister defect, delay time and defect growth*

Case	Initial defect	Growth	Delay time
“Reasonable estimate”	1 canister with 1 mm^2 1 ? m thin defect	Complete failure, i.e. a failure large enough (1 dm^2) not to offer any migration resistance, at delay time	$2\cdot10^5$ years
Pessimistic	5 canisters with the 1 mm^2 (i.e. 1 µm thin) defect	Complete failure, i.e. a failure large enough not to offer any migration resistance, after $2\cdot10^4$ yrs.	300 yrs
Variants	Failure in bottom	n.a.	"The water exclusion case" according to Bond *et al.* (1997).

5 Chemical and Physical Data

5.1 Groundwater chemistry - Reference waters

5.1.1 Source of information

Laaksoharju *et al.* (1998) identify reference waters for SR 97. The groundwater composition of these waters are taken from measurements at depth in four different boreholes selected to represent Aberg (KA S2:550-535), Beberg (KFI07:511-516 and BFI01:439-459) and Ceberg (KGI04:404-407). Using a principal component analysis and a qualitative discussion of the past hydrogeologic history of the sites Laaksoharju *et al.* (1998) suggest that these waters can be described in terms of mixing portions of e.g. meteoric water, biogenic water, sea water and brine groundwater. They also briefly evaluate the uncertainty, representativity and site spatial variability of these water compositions. In addition, Bruno *et al.* (1999) evaluate the interaction between groundwater and bentonite. This interaction will determine the chemistry in the bentonite pore water.

5.1.2 Use in SR 97

Groundwater composition is not directly used in the assessment model chain (see figure 3.1), but influences many of the analyses providing data to this chain. Groundwater composition is directly used in speciation calculations for pore-water chemistry and solubility calculations, see Bruno *et al.* (1997) and section 5.2 below. The groundwater composition is also used when selecting proper sorption and diffusion properties in the buffer (see Yu and Neretnieks, 1997 and section 5.3), in the backfill (see section 5.4) and in the far-field rock (see Ohlsson and Neretnieks (1997), section 5.5 and Carbol and Engkvist, 1997 and section 5.6). However, these properties usually only depends on macro properties. Diffusion data essentially only depends on ionic strength and sorption data essentially depends on redox, ionic strength and pH.

The conceptual model uncertainties in the use of water chemistry are discussed in the respective subsections mentioned here. Uncertainty in water chemistry itself is discussed in the next subsection, regardless of if it is conceptual or data uncertainty.

5.1.3 Uncertainties, correlations and dependencies on other parameters

The uncertainty in water chemistry itself concern

- measurement and sampling errors,

- representativity of water samples and spatial variability,
- development of water chemistry due to groundwater flow (i.e.) movement of groundwater with different chemistry,
- disturbance from the repository construction and operational phase,
- development of water chemistry due to interactions between the water and the rock and the engineered barriers.

Measurement and sampling errors

For the major components (Na^+, K^+, Mg^{2+}, HCO_3^-, Cl^- etc) the measurement errors are small in relation to the uncertainties discussed above. Laaksoharju *et al* (1998) report pure measurement errors of the major components to be in the order of 1-5 %. Errors are larger for trace elements (around 20% for Br^- and I^-, 50-100% for NO_3^-, NO_2^-, HN_4^-, PO_4^-) and even larger for isotopes. The relative uncertainty for pH and Eh measurements are in the order of 0.1 pH unit and 25mV, respectively, but the absolute errors introduced by difficulties with sampling are larger, especially for pH. Even if great care is taken to obtain undisturbed samples, pH can differ in the order of 0.3 units, or even up to 1 pH unit.

Spatial variability

Laaksoharju *et al.* (1998) selected the reference waters after careful examination of all water samples collected from the three SR 97 sites. The water samples selected are typical, at the respective sites, for the proposed repository depth. The different groundwaters explored at Aberg, Beberg and Ceberg respectively cover a wide range of chemical conditions from the high salinity, low carbonate and sulphate water of Aberg, the fresh low chloride and sulphate but high carbonate waters of Beberg to the fresh low carbonate, low chloride, low sulphate but high pH waters of Ceberg.

Water sampling implies bore hole penetration, which means that fully undisturbed conditions cannot be measured. However, care has been taken during measurement campaigns to exclude the risk of short circuits flow paths or other short term borehole disturbances. This is achieved by marking the drilling water and by sampling chemistry only after a prolonged pumping period. Usually, the chemical composition is constant during the pumping, implying a constant composition. However, an alternative interpretation is that the pumping imposes an artificial mixing of waters of different origin and type, thus masking a potential spatial variability in water chemistry.

By performing a statistical principal component analysis of the chemical data Laaksoharju *et al.* (1998) describe much of the variability of the data in terms of two principal components (i.e. different linear combinations of the water chemistry parameters). The main result, displayed in figure 5.1, gives a clear indication of the spatial variability of the water chemistry within each site and the difference in water chemistry between the three SR 97 sites.

Figure 5.1 indicates a strong variability at Aberg and a rather small variability at Ceberg, with Beberg somewhere in between. As shown in the figure, the analysis displays that most relevant water samples have compositions within the range of the four suggested reference waters, implying that the spatial variability at repository depth lies between these water compositions. Clearly, for Aberg there are also several water samples with compositions outside this range. These samples, however, were taken at depths below 1000 m or below the more shallow access tunnel passing below the sea where the water is strongly affected by the marine and biogenic surface conditions.

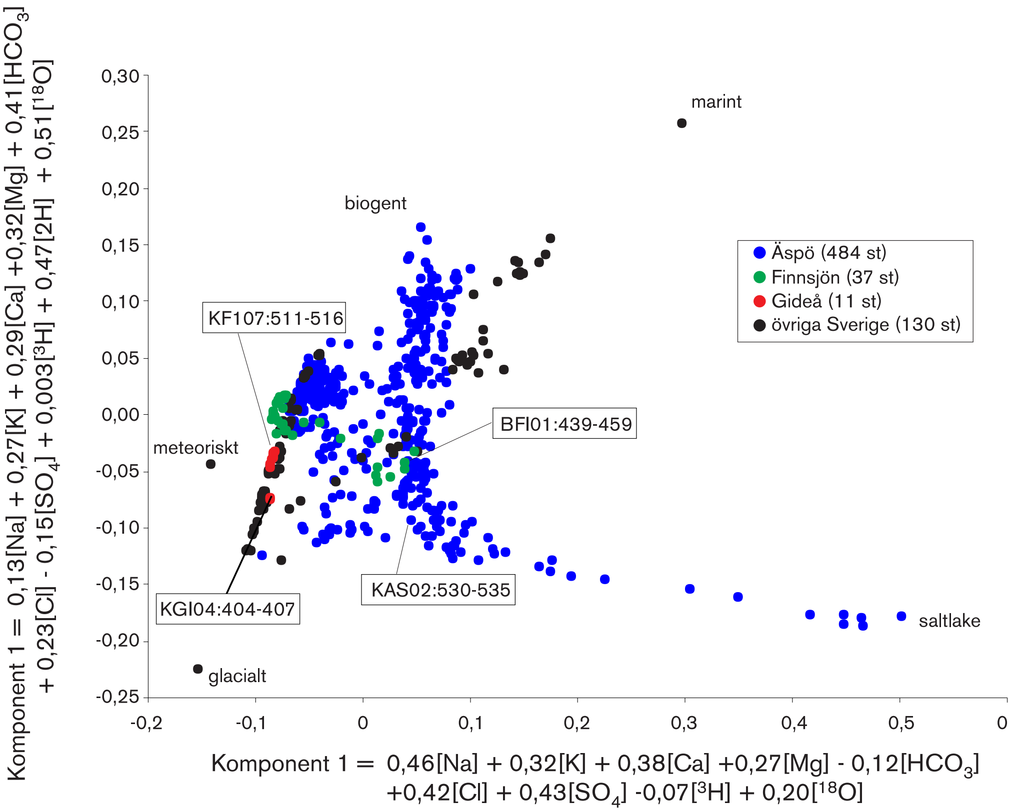


Figure 5.1 *Principal component analysis of all water samples taken from Aberg, Beberg and Ceberg as well as at other places in Sweden. The reference waters are indicated (from Laaksoharju et al.,* 1998*).*

Effect of groundwater movement

The effect of future groundwater movement is potentially important. Laaksoharju *et al.* (1998) show that present day water composition is a mixture of waters with different origin. However, the groundwater movement will continue also after sealing of the repository.

As land rise continues, the Aberg site, presently on an island close to shore, will become inland and the water chemistry will become less saline (Svensson, 1998).

However, the process is slow and is very much determined by the future climate state. Long term changes of the Aberg groundwater chemistry consequently lies outside the scope of the base and initial canister defect scenarios. (It will be considered in the climate scenarios).

At Beberg the transition from saline to fresh water conditions has proceeded a much longer time and at present both saline and non-saline water is found at the proposed repository depth (Hartley *et al*., 1998). If there is no climate change, it is likely that the saline water will disappear in the 5 000 year time frame, even if saline conditions cannot fully be excluded. For longer times, climatic changes need to be considered, but again this is outside the scope of the base and initial canister defect scenarios.

Despite the fact that also Ceberg, lies below the highest coastline, all water samples have no or, for some deep samples, very low salinity. It is most likely that the present high elevation of the site has allowed the past saline water to leave the system a long time ago. Present climate conditions does not suggest any alterations to these conditions.

Disturbance during construction and operational phase

During construction and operation there may be a risk that deep lying saline water will be drawn towards the repository through up-coning. The effect, if at all a problem, is strongly dependent on the repository construction and could possibly be handled by proper engineering. The presence of oxygen and different organic material during construction and operation may also affect the local water chemistry, but again the effect depends on the details of the repository construction. It is anyway likely that bacteria will rapidly consume the oxygen. The initial state of the repository is further evaluated under the framework of the base case scenario of SR 97.

Interaction with rock and engineered barriers

The interaction with the rock minerals is insignificant in the time span of interest.

Regarding the water chemistry in the bentonite pore water Bruno *et al.* (1999) suggest that the transition from ”pure” bentonite water to ”rock” water among other things depends on the rock water composition and could take considerable time for Ceberg. This needs to be considered when selecting solubilities and sorption properties in the buffer (see sections 5.2 and 5.3).

5.1.4 Quantification of uncertainties

The *reasonable* water chemistries are obviously the reference water chemistries provided for the different sites. For Beberg it is likely that the water eventually will become fresh and thus the low ionic strength KFI07 water should be selected, even if the saline case needs to be retained for the uncertainty evaluation (see below). In the buffer, however, it is necessary to consider the interaction between the bentonite and the groundwater (this is discussed in sections 5.2 and 5.3).

Given the spatial variability and even the more short range uncertainty in water chemistry discussed above, it seems reasonable to represent the uncertainty and the spatial variability in water chemistry by the range (in water chemistries) represented by the four reference waters. This possible range in groundwater composition should be considered when discussing probabilistic calculation cases for parameters (i.e. solubility, sorption and diffusivity, see remaining subsections in this chapter), which directly depend on water chemistry.

Water chemistry affects performance parameters such as solubility and sorption in different ways, which makes it impossible to directly nominate a *pessimistic* water chemistry. Instead the approach suggested is to select the water chemistry in the range of reference waters in Laaksoharju *et al*. (1998) and buffer pore water, which will produce the most pessimistic solubility, diffusivity or sorption coefficients.

Table 5.1.1 summarises the above recommendations.

Table 5.1.1: *Suggested quantification of uncertainty in water chemistry*

Case	**Aberg**	**Beberg**	**Ceberg**
Reasonable estimate	Reference water for Aberg in Laaksoharju *et al*. (1998), but consideration of different buffer pore water (see 5.2 and 5.3)	Reference water for Beberg (KFI07) in Laaksoharju *et al*. (1998), but consideration of different buffer pore water (see 5.2 and 5.3)	Reference water for Ceberg in Laaksoharju *et al*. (1998), but consideration of different buffer pore water (see 5.2 and 5.3)
Pessimistic	Select the water chemistry in the range of reference waters in Laaksoharju *et al*. (1998) and buffer pore water, which will produce the most pessimistic solubility, diffusivity or sorption coefficients.	Select the water chemistry in the range of reference waters in Laaksoharju *et al*. (1998) and buffer pore water, which will produce the most pessimistic solubility, diffusivity or sorption coefficients.	Select the water chemistry in the range of reference waters in Laaksoharju *et al*. (1998) and buffer pore water, which will produce the most pessimistic solubility, diffusivity or sorption coefficients.

5.2 Solubilities

5.2.1 Source of information

Bruno *et al.* (1997) have performed solubility calculations and also discuss uncertainties in the estimates. The calculations are made for the Aberg, Beberg and Ceberg reference waters (see section 5.1 and Laaksoharju *et al*, 1998) using the speciation code EQ3NR (Wolery, 1992), with a correction for the ionic strength of the system using the b-dot equation (Helgeson, 1969). For Beberg only the ”fresh” reference water is used as the saline Aberg water is assumed to be a fair representation of the Beberg saline water. In addition, a *bentonite pore water* has been evaluated. The pore water (Wanner *et al.*, 1992) is not related to site specific water compositions. In addition, Bruno *et al.* (1997) evaluates solubilties for a range of pH, pe, carbonate and temperatures.

The original thermodynamic data used has been taken from the NTB91-07 and 91-08 databases developed by Nagra. Uranium data from Puigdomenech and Bruno (1988), plutonium data from Puigdomenech and Bruno (1991) and REE data from Spahiu and Bruno (1995) have been used. Bruno *et al.* (1997) have, however, modified these data in a manner discussed in the report.

The basic principle has been that the less crystalline metal hydroxide phases are kinetically favoured and consequently constitute the initial solubility limiting phases (Ostwald Principle). As an alternative Bruno *et al.* (1997) also present results based on the possibility that Ra is solubility limited by co-precipitation with other alkaline-earth elements, and for curium and americium that their solubilities are limited by co-dissolution from the fuel according to the lower concentrations measured in spent fuel leaching tests. The co-precipitation approach has also been applied in calculations for Ni.

5.2.2 Use in SR 97, modelling approach and conceptual model uncertainties

Solubilities are used in the near-field source term code COMP23 where elements dissolve or precipitate in the canister compartment depending on the concentration in the respective compartments. Precipitation could not occur in a compartment further out. This simplification also implies that high solubilities would always lead to higher releases. Each isotope of an element could use the full solubility even if there are other isotopes of the same element available (i.e. COMP23 does not split the total solubility between isotopes). This is a pessimistic assumption. Furthermore, the ongoing corrosion of the steel canister will most likely ensure reducing conditions inside the canister, which implies that the solubilities recommended by Bruno et al. (1997) also can be used for conditions inside the canister. Bruno et al., (1999) explores, in more detail, the water chemistry inside a broken canister.

The calculation of the solubilities also assumes that the redox state of the elements are reversible. As pointed out in the “process report” (SKB, 1999), this is true for most elements but probably not for Se. The validity of the Se results would then depend on the redox state of Se in the spent fuel and its potential oxidation during fuel conversion. This means that pessimistically one would need to assume an oxidising state of Se, leading to essentially infinite solubility.

For the modelling of solubility values, see the above section.

Bruno *et al.* (1997) discuss the following conceptual model uncertainties with the approach adopted for calculating solubilities:

- uncertainties in dissolution/precipitation mechanisms and in particular the possibilities for co-precipitation and co-dissolution,
- uncertainties in transient behaviour versus the equilibrium analysis assumed and uncertainties in the identification of the solubility limiting solid phase,
- influence of groundwaters at high ionic strength,
- EQ3NR only allows that a solid phase can be equilibrated with one component

The potential importance of co-precipitation/dissolution is analysed by alternatively considering these mechanisms for Ni, Ra, Am and Cm (see next section).

Bruno *et al.* (1997) note that EQ3NR is a speciation solubility code for modelling the thermodynamic state of an aqueous solution. It involves a static calculation based on water chemistry and analysis. These kind of models are better used when they are employed to test the degree of dis-equilibrium of heterogeneous reactions than when they are forced to assume that such reactions are in equilibrium, which is the application needed in performance assessment. This problem is handled by selecting the least favourable solubility limiting phase among a set of many different analysed phases. This leads to an overestimation of the actual solubilities. For some elements Bruno *et al.* (1997) compare solubilities with naturally occurring concentrations, implying that in reality the concentrations of some elements may be much lower and thus controlled by other phases.

The influence of ionic strength is handled by using the b-dot equation (Helgeson, 1969), which is used by default by the EQ3NR code. Bruno *et al.* (1997) consider this as sufficiently accurate taking into account the relatively low ionic strength of the groundwaters considered.

Another limitation of the model found during calculations and discussed by Bruno *et al.* (1997) has been that a solid phase can only be equilibrated with one component, i.e., one cannot equilibrate calcite with calcium and carbonate at the same time, in the same input. This fact is an important constraint when simulating heterogeneous equilibria in natural systems. To solve this limitation, Bruno *et al.* (1997) suggest that one can precipitate calcite until equilibrium with the EQ6 code package, otherwise in such case, pH could not be maintained fixed during the calculation.

5.2.3 Data uncertainties, correlations and dependencies on other parameters

Bruno *et al.* (1997) address the following sources of data uncertainty in solubility data provided for performance assessment:

- influence by temperature on thermodynamic data,
- other uncertainties in the thermodynamic data,

- uncertainties in dissolution/precipitation mechanisms and in particular the possibilities for co-precipitation and co-dissolution,

- uncertainties in groundwater composition.

The thermodynamic data used represent room temperature (25 °C). Bruno *et al.* (1997) evaluate the influence of temperature for ten radionuclides for which thermodynamic data at 15 and 60 °C were available. They observed up to a factor of 10 variation compared to the 25 °C data (up to 100% coefficient of variation in log scale).

Bruno *et al.* (1997) treat the uncertainty in thermodynamic data by a careful evaluation of the data used and selection of aqueous complexes and limiting solid phases relevant to the conditions of interest. In general, it is noted that the uncertainties associated with the thermodynamic data are primarily related to the availability of this information. A lack of information has been found related to the dependency on temperature of the thermodynamic data as temperature dependent data only were available for ten radionuclides. Another important source of uncertainty in the solubilities is associated with the accuracy and consistency of the thermodynamic data available. It is noted that evaluating the accuracy of thermodynamic data is a complex task, as evidenced by the NEA/OECD effort in compiling a selected set of consistent thermodynamic data for inorganic aqueous species and solid phases of uranium (Grenthe *et al.*, 1992) and americium (Silva *et al.*, 1995). Because such evaluations are unavailable for many radionuclides Bruno *et al.* (1997) suggest an uncertainty of ±0.5 logarithmic units in solubility calculations associated with the inaccuracy of thermodynamic data.

The potential importance of co-precipitation/dissolution is analysed by alternatively considering these mechanisms for Ni, Ra, Am and Cm. It is well established that Cm co-precipitates with Am, but the significance of co-precipitation of the other elements is less well established. In addition, there are also other mechanism controlling the actual precipitation/dissolution process (SKB, 1999). For consequence calculations there seems to be few alternatives but to use thermodynamic equilibrium data and assumptions. It should be kept in mind, though, that such an approach leads to pessimistically high solubilities.

The uncertainty in groundwater composition is handled by evaluating solubilities for the different groundwater compositions for Aberg, Beberg (only the fresh from KFI07) and Ceberg given by Laaksoharju *et al.* (1998) and for a bentonite water with a composition given by table 7-3 in Bruno *et al.* (1997). The results of the calculations are provided in table 7-4 (bentonite values) and table 9-4 in Bruno *et al.* (1997) and summarised in table A.2.2.2. Table A.2.2.2 only shows the solubilities for the species resulting in the highest solubilities.

In addition, Bruno *et al.* *(*1997) present a sensitivity analysis of the impact of uncertainty in groundwater composition exploring the impact of pH (from 7 to 9) , carbonate (10^{-4} to $5{\cdot}10^{-3}$), pe (-5.21 to -1) and temperature (15 °C and 60 °C). Table A.2.2.2 (using table 11-7 in Bruno *et al.*, 1997) also present the results of these calculations. This variation, however, only partly cover the difference between the different waters analysed. In fact, as previously stated, the water compositions analysed span a wide spectrum from the high salinity, low carbonate and low sulphate water of

Aberg, the fresh low chloride and low sulphate but high carbonate waters of Beberg to the fresh low carbonate, low chloride, low sulphate but high pH waters of Ceberg. The sensitivity analyses, however, consider smaller pH values (down to 7), which turn out to be of major significance for some nuclides. The wider range in pe, which still is within the reducing region, has far less importance.

Table A.2.2.2 also states infinite solubility for Se for the pessimistic case, in order to account for the uncertainty in the redox state of Se, as discussed above.

As discussed in section 5.1 the uncertainty in groundwater composition both refer to the temporal and spatial variability of the rock groundwater chemistry and the transient equilibration of the bentonite porewater with the ”rock” groundwater. The development of the latter is analysed by Bruno *et al.* (1999) and it shows that the transition from ”pure” bentonite water to ”rock” water among other things depends on the rock water composition and could take considerable time for Ceberg. The bentonite water used for solubility calculations is not based on the actual water compositions of the different sites, but it is still fair to assume that the actual water composition would lie somewhere between the site waters and the bentonite waters.

Bruno *et al.* (1997) notes the following from their calculated results:

- The low carbonate content of Ceberg results in a comparably low solubility of Ni. However, sensitivity analyses with COMP23 shows that all Ni solubilities are so high that the release probably is not limited by solubility anyway.

- The considerable differences in Ag solubilities are due to the fact that AgCl(s) was considered as solubility controlling solid phase for the A-, Be- Ceberg calculations. The extremely low solubility calculated for the bentonite waters should not be used. (Scoping calculations show that Ag is totally irrelevant for the release calculations though).

- The Ra solubility is much higher for Ceberg due to its low sulphate content.

- The Th solubility is higher at Beberg and in the bentonite water due to the phosphate content and the high pH.

- The Np solubility is higher at Beberg due to the phosphate content.

- The Pu solubility is higher at Aberg due to its pH sensitivity.

- The Am solubility is slightly higher at Aberg mainly due to the lower pH.

The sensitivity analysis by Bruno *et al.* (1997) essentially confirms these trends. However, they analyse even lower pH which results in an even higher pH sensitivity for Pu, Ni, Cm, Am, Se, and Sa, which all have the highest solubility calculated for pH=7, as can be seen from table A.2.2.2. The effect is particularly significant for Pu which increases its solubility by 4 orders of magnitude if pH drops from 7.7 (the Aberg reference water) to 7. This explains the large range in the last column in table 5.2.1 compared to the difference in Pu solubility between the different reference waters.

These results show that many uncertainties in solubilities of different elements are inter correlated since much of uncertainty depends on uncertainty in groundwater composition. pH, carbonate, phosphate and redox conditions seem to be the most important factors.

5.2.4 Quantification of uncertainties

It appears that the uncertainties associated with co-precipitation and selection of solubility controlling solid phases still makes it necessary to select the phases leading to the highest solubility also for the *reasonable* solubility. Given the long time before releases could be expected it also appears sensible to select solubilities calculated for the prescribed water chemistry of Aberg, Beberg and Ceberg as reasonable estimates assuming that Beberg will be fresh in the long run. Furthermore, as already noted, it is fair to assume that the actual water composition would lie somewhere between the site waters and the bentonite waters. Given the lack of more detailed evaluations it is thus suggested to select the *reasonable estimate* solubility at a site as the maximum of the solubility in the rock water of that site and the bentonite solubility.

One approach to derive a pessimistic case, with respect to uncertainty in groundwater composition, is to select the groundwater composition in table A.2.2.2 (Aberg, Beberg, Ceberg or bentonite) leading to the highest ”total” release. However, inspection of table A.2.2.2 does not directly suggest such a case. A more extreme *pessimistic case* would be to select the highest solubility of each element regardless of the consistency in water chemistry including the uncertainty range provided by Bruno *et al. (*1997). Given the expected evolution of the groundwaters and the different time scales involved for the different elements this approach may not be as far fetched as it may appear, i.e. the variations *between* sites, as seen today, may in fact reflect variations *within* sites in the future. The solubility of Se should be put to infinity for the *pessimistic* case, as already discussed.

There seem to be little reason to analyse the high pe solubilities for the canister defect scenario. The numbers should be used in sensitivity analyses and possibly for other scenarios.

Table 5.2.1 summarises the above suggestions.

Table 5.2.1: *Suggested quantification of uncertainty in solubility*

Case	Aberg	Beberg	Ceberg
Reasonable estimate	See table A.2.2.3. The highest of the Aberg solubility and the bentonite solubility of table A.2.2.2 Table A.2.2.2 is based on the highest for Äspö (Aberg) in table 9-4 in Bruno *et al.* (1997).	See table A.2.2.3. The highest of the Beberg solubility and the bentonite solubility of table A.2.2.2 Table A.2.2.2 is based on the highest for Finnsjön (Beberg) in table 9-4 in Bruno *et al.* (1997).	See table A.2.2.3. The highest of the Ceberg solubility and the bentonite solubility of table A.2.2.2 Table A.2.2.2 is based on the highest for Gideå (Ceberg) in table 9-4 in Bruno *et al.* (1997).
Pessimistic	See table A.2.2.3 (based on the highest for each element in table 7-4 (bentonite), table 9-4 and table 11-7 in Bruno *et al.* (1997).	See table A.2.2.3 (based on the highest for each element in table 7-4 (bentonite), table 9-4 and table 11-7 in Bruno *et al.* (1997).	See table A.2.2.3 (based on the highest for each element in table 7-4 (bentonite), table 9-4 and table 11-7 in Bruno *et al.* (1997).

5.3 Sorption and diffusivity in bentonite

5.3.1 Source of information

Yu and Neretnieks (1997), compile published measurements of diffusion and sorption properties in water saturated compacted bentonite, critically review sources of errors and recommend values for use in performance assessment. Ochs (1997) has reviewed the work by Yu and Neretnieks and also explicitly addresses uncertainty in the values. All suggested values refer to an MX 80 bentonite, for a dry compaction density of 1590kg/m^3, a wet density of 2000 kg/m^3 and a porosity ε=0.41, which is in accordance with the specification given by Bäckblom (1996). No other composition will be evaluated quantitatively within SR 97.

5.3.2 Use in SR 97, modelling approach and conceptual model uncertainties

SR 97 models migration through the buffer by diffusion and sorption. The near-field release code COMP23 uses a ”lump-sum” parameter approach describing these processes with nuclide (or rather element) specific values for distribution coefficients K_d, effective diffusivity D_e, and porosity ε.

For most elements porosity is given by the bentonite specification, but some elements require a lower porosity in order to handle ion exclusion. In practice, this poses a problem in COMP23, which only can handle a single porosity. This is handled by adopting the low porosity for all elements and then readjust the K_d values for the non ion-exclusion elements such that the sorption capacity would equal the sorption capacity using the ”real” K_d values and the high porosity. The D_e values are not readjusted accordingly, but the impact of such a change would be quite minor and the errors can thus be disregarded.

Yu and Neretnieks (1997) discuss the need for more complex diffusion and sorption models including surface diffusion. Ochs (1997) conclude that the K_d values cannot be evaluated independently of the diffusion model used. For example, applying a more complex model, such as the surface diffusion model, may potentially result in higher K_d values for Cs. Such a value could, however, not be used before also changing the assessment migration model to handle surface diffusion. In SR 97 COMP23 applies a traditional diffusion model implying that the sorption and diffusivity data assembled under this hypothesis are consistent with the assessment model used.

5.3.3 Data uncertainties, correlations and dependencies on other parameters

The following discussion of uncertainties builds on Ochs (1997).

Very few sorption and diffusion experiments have been carried out at elevated temperatures and it is thus difficult to quantify the effect. There is a lack of basic chemical data. In general, sorption will decrease and diffusion increase with temperature, but the uncertainties with predicted chemical conditions in the buffer and with the speciation of many elements are probably much more relevant.

Experimental uncertainties are discussed by Yu and Neretnieks (1997) and are generally considered in the range of values given. However, there is reason to be critical to K_d-values measured in batch experiments with very low bentonite/water ratios. In contrast D_a values are measured in bentonite at relatively high dry densities. Soluble impurities contained in the bentonite will lead to relatively high concentrations of dissolved salts in compacted bentonite (see also the paragraphs below). Thus direct application of ”fresh” water K_d:s is not valid.

The migration characteristics strongly depend on the bentonite pore water composition and mainly on the following:

- Redox conditions affect redox sensitive elements (C, Np, Pa, Pd, Pu, Se, Tc and U).
- Solution pH highly affect sorption of elements (Am, Ce, Nb, Ni, Np, Pa, Pb, Pd, Pu, Sm, Sn, U, Zr) that exists as hydrolysed cations around the neutral pH range. Usually the pH influence is critical if pH is below 6 as this implies changes in the sorption process. Other elements (Cs, Ra, Sr) sorb via ion-exchange reactions and are in practice not influenced by pH. The apparent diffusivity may change as a function of D_a.
- Apart from redox and pH the concentration of dissolved ligands in the bentonite porewater affects sorption and diffusion behaviour.

Ochs (1997) claims that a critical evaluation of the data proposed by Yu and Neretnieks (1997) is made difficult by the fact that they are not attached to a well defined pore water reference system.

Ochs (1997) modelled the porewater composition by allowing two reference groundwater (Äspö KAS02 saline and Finnsjön KFI07 fresh, see section 5.1 and Laaksoharju *et al.*, 1998) to equilibrate with the MX-80 bentonite. From this the following conclusion can be drawn:

- the influence of fresh and saline groundwater on porewater composition may be quite small when considering soluble impurities (e.g. $CaSO_4$ and NaCl) in the bentonite to be dissolved resulting in ”saline” pore waters regardless of rock water composition

- pH may be around 7 or lower, but allowing CO_2 to escape would result in a pH slightly above 8.

In fact, independent evaluation of the bentonite porewater chemistry conducted by Bruno *et al.* (1999, see section 5.1) generally supports these conclusions. They suggest that the transition from ”pure” bentonite water to ”rock” water among other things depends on the rock water composition and could take considerable time for Ceberg, where pH in the buffer, occasionally, could be as high as 11.

Ochs (1997) also discusses these influences in detail for each element considered. Based on his suggestions a modified table of values, compared to Yu and Neretnieks (1997), can be produced (table A.2.3.3). This table, in turn, can be used to select migration parameters for a reasonable and a pessimistic case as discussed in the next sub-section.

5.3.4 Quantification of uncertainties

Based on the discussion of Ochs (1997) the following approach is suggested for SR 97:

- Given the ionic strength of the porewater one should only use the ”saline” data in table 5.3.1 this is also supported by the evaluation by Bruno *et al.*, 1999.

- It is fair to assume that CO_2 will escape and thus safeguard a pH above 8. This means that the lower range of validity of the data in table 5.3.1 will not be breached. However, the evaluations made by Bruno *et al.* *(*1999) suggest that the pH resulting from interaction with Gideå water would be around 11, *i.e.* above the range of validity for the data (pH 8-10). This violation of the pH range is less dramatic than a breach in the lower end, as there will be no change in sorption mechanisms, but warrants further studies of K_d at high pH. Since no dramatic effect are expected such studies can be conducted outside SR 97.

- Given the studies concerning the buffering capacity of the bentonite (Bruno *et al.*, 1999) and the huge amount of iron in the canisters only the ”reducing” data in table 5.3.1 are applicable for the initial canister defect scenario analysis.

- The effect of elevated temperatures should be explored, but given the likely limited impact of temperature such studies can be conducted outside SR 97.

- Yu and Neretnieks do not present values for Ag, Cm and Ho. In reality, this is of little importance due to the low abundance of these elements, but numbers need nevertheless to be supplied. It is here suggested to use zero K_d for Ag, use the Am values for Cm and Sm values for Ho.

Based on this approach the following is suggested. The *reasonable estimate* should be the *reasonable estimate* values for saline and reducing in table A.2.3.3. The pessimistic values would be the pessimistic values for saline and reducing in table A.2.3.3. When available the values suggested by Ochs should be used, otherwise one should apply the values suggested by Yu and Neretnieks (1997).

The conclusions are summarised in table 5.3.1, and the resulting parameter values are summarised in table A.2.3.2.

Table 5.3.1 *Suggested quantification of uncertainty in buffer migration data*

Case	Description
Reasonable estimate	See table A.2.3.2 (based on reasonable estimate values for saline and reducing in table A.2.3.3)
Pessimistic	See table A.2.3.2 (based on pessimistic values for saline and reducing in table A.2..3.3)

5.4 Sorption and diffusivity in backfill

5.4.1 Source of information

In SR 97 it is assumed that the backfill will consist of a crushed rock/bentonite mixture containing 15% bentonite (Bäckblom, 1996). There are no specific migration data on the backfill, but it is suggested that reasonable parameter values can be deduced by combing migration data of the buffer (see section 5.3) and of the crystalline rock (see section 5.6).

5.4.2 Use in SR 97, modelling approach and conceptual model uncertainties

SR 97 models migration through the backfill by diffusion and sorption, i.e. the same as in the buffer. The near-field release code COMP23 uses a ”lump-sum” parameter approach describing these processes with nuclide (or rather element) specific values for distribution coefficients K_d, effective diffusivity D_e, and porosity ε.

The backfill analysed in SR 97 will contain 15% bentonite and 85% crushed rock. A simplistic approach to obtain K_d values for the backfill is to make a weighted average of 15% bentonite K_d-values and 85% crushed rock K_d-values. Yu and Neretknieks (1997) provide K_d-values for bentonite as already discussed in the previous section. The K_d-

values for rock, as presented by Carbol and Engkvist (1997) can be used for the crushed rock as well. Porosity will be similar to bentonite (30%), but due to the dilute clay it is assumed that there is no ion-exclusion effect in the backfill. This means that all ions are assumed to have an effective diffusivity of 10^{-10} m^2/s with a porosity fixed to 30% .

Since sorption in the backfill is attributed to both the bentonite and the rock, the uncertainties in bentonite migration properties and the uncertainties in the rock properties also apply for the backfill. In addition, the following may be worth to mention:

The backfill will contain dilute bentonite. Thus, the chemical buffering capacity would not be as pronounced and the pore water chemistry in the backfill be will more close to the rock groundwater chemistry. If needed, the consequence of dilute bentonite could be handled by also using the low salinity values provided by Yu and Neretnieks (1997).

The hydraulic conductivity of the backfill may be in the order of 10^{-10} m/s or higher, which is not significantly less than the hydraulic conductivity of the surrounding rock mass. This implies that there may be groundwater flow in the backfill although other factors, such as plugs, need to be considered as well. In order to address this problem Pettersson et al., (1999) explores the potential effects of flow in the backfill by a special model exercise. Moreno concludes that the impact of flow has little influence on the release since the main transport resistance in the near-field is not located in the tunnel. If the canister damage is small the release will be controlled by the release through the hole, for larger canister damage the bentonite buffer will control the release. At most the release increase by a factor of two for a few nuclides.

5.4.3 Data uncertainties, correlations and dependencies on other parameters

For a more elaborate discussion on uncertainties in backfill K_d values, see section 5.3 and for the rock K_d-values, see section 5.6. However, for the backfill it seems appropriate to consider the low salinity values for the low salinity rock groundwaters (i.e. Beberg fresh and Ceberg fresh) since the bentonite will only occur in a diluted form. Table A.2.4.2 shows the K_d values resulting from a the proportional contribution of 15% of bentonite values as suggested by Yu and Neretnieks (1997) and 85% rock values as suggested by Carbol and Engkvist (1997). Realistic values for bentonite are combined with the realistic values for rock etc.

The backfill diffusivity (and porosity) may show strong spatial variability due to the practice of the emplacement techniques. Such problems, however, lie outside the scope of the canister defect scenario of SR 97.

Finally, it is evident that the suggested handling of migration properties is relatively simplistic. However, the approach can certainly be motivated in light of scoping release calculations carried out (Hedin, *pers. comm.).* They suggest in fact, that neither backfill sorption nor diffusivity are important parameters for the release and near-field migration.

5.4.4 Quantification of uncertainties

As motivated in the previous section a *reasonable estimate* for the backfill diffusivity would be 10^{-10} m^2/s. Reasonable estimate values for K_d should be based on a proportional contribution from 15% bentonite and 85% crushed rock for the reasonable estimate water chemistries. This implies selecting saline reducing values for Aberg, fresh reducing values for Beberg and fresh reducing values for Ceberg from table A.2.4.2. However, given the relative insignificance of the buffer on one hand and the uncertainty regarding flow and buffer composition it may be motivated just to select the pessimistic values, see next paragraph.

Pessimistic values for K_d could be selected from the pessimistic column of table A.2.4.2. Only the ”saline” values should be used to avoid motivation of the water chemistry. The diffusivity value 10^{-10} m^2/s is already close to free water diffusivity. The backfill diffusivity will have very little impact on results. Consequently it is suggested not to change diffusivity for the pessimistic case.

Table 5.4.1 summarises the suggestions given above.

Table 5.4.1: *Suggested quantification of uncertainties in backfill sorption and diffusivities*

Case	*Aberg*	*Beberg*	*Ceberg*
Reasonable estimate	D_e 10^{-10} m^2/s, saline K_d from Table A.2.4.2 ε= 0.30	D_e 10^{-10} m^2/s, fresh K_d from Table A.2.4.2 ε= 0.30	D_e 10^{-10} m^2/s, fresh K_d from Table A.2.4.2 ε= 0.30
Pessimistic	D_e 10^{-10} m^2/s K_d from Table A.2.4.2, pessimistic, saline ε= 0.30	D_e 10^{-10} m^2/s K_d from Table A.2.4.2, pessimistic, saline ε= 0.30	D_e 10^{-10} m^2/s K_d from Table A.2.4.2, pessimistic saline. ε= 0.30

5.5 Matrix porosity and diffusivity

5.5.1 Source of information

Ohlsson and Neretnieks (1997) recommend nuclide specific diffusion data in granite and also discuss uncertainties. The recommendations are based on diffusion experiments with tritiated water (HTO) and some cations in salty water in the same rock samples from Äspö (i.e. Aberg) conducted by Johansson *et al.* (1996). Diffusivities for other nuclides are assessed from their theoretical relation to the HTO diffusivity by considering differences in free water diffusivities and possibilities for anion exclusions or surface diffusion.

5.5.2 Use in SR 97, modelling approach and conceptual model uncertainties

Matrix porosity and diffusivity are used in the far-field migration code FARF31 to describe diffusion in the rock matrix. This model assumes that there exist an interconnected pore space inside the rock matrix and models migration as a diffusion process retarded by sorption on the rock matrix itself. FARF31 uses an ”effective” diffusivity” D_e, which takes care of the combined effect of porosity and diffusion in the interconnected pore space.

Ohlsson and Neretnieks (1997) do not discuss the validity of the matrix diffusion model itself, but rather concentrate on the uncertainty of the data to this model. They do, however, consider the fact that diffusion inside the matrix can be nuclide specific. This is due to differences in free water diffusivities, possibilities for anion exclusion and surface diffusion.

Inside the matrix the diffusion process is essentially controlled by the ”apparent diffusivity, i.e. the ratio $D_a=D_e/(\varepsilon+\rho K_d)$. However, the impact of the matrix diffusivity on breakthrough time for a specie dissolved in the flowing water of a fracture is controlled by the product $D_eK_d\rho$ (Ohlsson and Neretnieks, 1997) as the exchange between the flowing water and the matrix is proportional to $a_r/q{*}D_e$. Consequently, the retardation increases for high values of D_e and K_d and decreases for low values (in contrast to $1/D_a$ which decreases for high K_d:s).

5.5.3 Data uncertainties, correlations and dependencies on other parameters

The data uncertainty regarding porosity and diffusivity essential concern

- spatial variability of porosity,
- impact of groundwater chemistry on the nuclide specific diffusivities.

Regarding porosity, the basic assumption made is that a non-interacting species will have an effective diffusivity that is less than in pure water by a factor equal to a rock property called the *formation factor* accounting for porosity and tortuosity. The proposed formation factor for Swedish rock is reported to $4.2\ 10^{-5}$ for a porosity of 0.5 %. This value is based on measurements on samples (1-2 cm) of the Äspö diorite used for through diffusion experiments by Johansson *et al.* (1996).

The formation factor and porosity considered reflect Aberg pristine rock, i.e. rock that does not contain weathered surfaces or is close to any fractures. Values specific to Beberg or Ceberg are not provided. Ohlsson and Neretnieks (1997) note that investigations of materials containing fracture surfaces mostly display larger porosity and diffusivity. They state that porosity variations between 0.1% and 1% are common in granitic type rock, but do not comment whether this variability is inter or intra site ”dominant”. Furthermore, Ohlsson and Neretnieks do not discuss porosity variability perpendicular to the flowing fracture.

It has been suggested, e.g. Nagra (1994, p 239) that the interconnected pore space only concern a limited region close to the fracture. Furthermore, diffusion experiments are carried out in a laboratory scale implying migration distances on the order of centimeters implying that there may be an uncertainty concerning the connectivity of the pore structure over longer distances. However, for example SKI, (1991) demonstrate that for sorbing nuclides a penetration depth in the order of 10^{-3} m is almost indistinguishable to unlimited potential penetration. Furthermore, Ohlsson and Neretnieks (1997) discuss porosity of pristine rock, outside the vicinity of fractures, which seem to be pessimistic as this would mean that they do not take into account potential increase in porosity close to the fractures.

It may also be questioned if diffusivities and porosity measured in laboratory are affected by the reduction of rock stress, which may result in an increase in porosity. However, comparison between laboratory data and results of in-situ in-diffusion experiments carried out in boreholes (Skagius and Neretnieks, 1986), suggest that this is a factor of 2 effect only. The issue may not be closed, but appears to be sufficiently bounded for the needs of SR 97.

In conclusion, it still appears evident that the formation factor has an order of magnitude natural variability even in locations close to each other. In fact diffusion coefficients differ by factors of 10-100 or more in different studies. However, as showed in appendix 2 of Ohlsson and Neretnieks (1997), variability along a flow path may not have a major influence since the system is close to linear and the variations are averaged out. Still an overall factor of 10 reduction of the reasonable estimate porosity does not seem unfair for a pessimistic case.

Regarding diffusivity Ohlsson and Neretnieks only use direct measurement of the HTO diffusivity, which is assumed to be non-interacting. The effective diffusivities for other species are obtained by proportioning with the respective diffusivities of free water. This gives a correction factor of 2-3.

In low ionic strength waters anions, such as iodide, chloride, pertechnetate etc., have lower effective diffusivities by one order of magnitude due to anion exclusion. Also in low ionic strength waters some cations, such as Cs, Sr and Na, have an effective diffusion coefficient that is one to two orders of magnitude higher than that of tritium due to surface diffusion. In practice Ohlsson and Neretnieks suggest to divide diffusivities with a factor of 10 for anion exclusion and to increase it by a factor 10 for surface sorption species. One should remember though that increasing diffusivity implies increased retention capacity. However, the factor of 10 increase suggested, is supposed to be small in relation to experimental values. Surface diffusion is further described by e.g. Glover *et al.* (1994) and Revil and Glover (1998).

Ohlsson and Neretnieks (1997) consider waters as *high ionic strength* if the salt concentration is above 10 000 mg/l. For the SR 97 waters, this apparently applies for Aberg and the saline Beberg waters (TDS is 11 107 mg/l for Aberg and 9457 mg/l for Beberg/saline, see Laaksoharju *et al.*, 1998). *Low salinity waters* refer to waters with a salt concentration less than 1000 mg/l. For the SR 97 waters, this apparently applies to Ceberg (TDS is 338 mg/l and possibly Beberg/fresh TDS 1339 mg/l). Waters in the intermediate range are not discussed.

The following conclusions can be drawn:

- Diffusivities show strong spatial variability due to spatial variability in formation factor. Clearly, the spatial variability as such is not an uncertainty but a site property (see the principal discussion in section 2). However, since the location of the failed canisters and the location of migration paths is unknown one would need to consider that migration paths sample a significant portion of the spatial variability. This will result in uncertainty in migration path properties. Much of the spatial variability is averaged out along migration path, but there does not seem to exist a careful analysis of the spatial correlation structure of diffusivities. Evidently, the effect of spatial averaging would depend on this structure.

- Diffusivities of ions are affected by the ionic strength. The effect appears to be at least one order of magnitude effect.

In order to account for these uncertainties Ohlsson and Neretnieks (1997) suggest to use the nuclide and salinity specific diffusivities and to apply an overall factor of 3-5 uncertainty for high saline water and an overall factor of 10 uncertainty for the charged species for low ionic strength waters. It should also be noted that given the fact that only the square root of D_e affect migration only order of magnitude uncertainties really matter.

In addition to changes of the diffusivities due to anion exclusion, for the low ionic strength waters, it could be debated if also matrix porosity should be adjusted accordingly for the anions. This is not discussed by Ohlsson and Neretnieks (1997) but has been assumed in the TVO-92 (Vieno *et al.*, 1992) and TILA-96 (Vieno and Nordman, 1996) safety assessments carried out in Finland. According to Olin *et al.* (1996) diffusion experiments in different crystalline rock samples suggest that only a fraction of the pore volume is open to anions while the rest is open only to cations and neutral species. It should be noted that changes of matrix porosity only affects the transient diffusion of non-sorbing species and is not of major importance for the safety assessment results. For sorbing species the migration is controlled by the effective diffusivity D_e, as already discussed, and by the sorption coefficient. Nevertheless it is important to apply consistent parameter sets in the analysis. Consequently it is suggested to reduce the porosity parameter in the assessment code with a factor of 10 for the anions where effective diffusivity is reduced.

5.5.4 Quantification of uncertainties

As a *reasonable estimate* it appears well founded to directly use the diffusivities specified in table 2 of Ohlsson and Neretnieks (1997) with ”High” for Aberg and ”Low” for Beberg and Ceberg (assuming that Beberg will eventually become fresh at the time of release see section 5.1). Apart from Na and Sr this will also generally result in lower, i.e. more pessimistic, diffusivities for Beberg.

As a *pessimistic case* Ohlsson and Neretnieks suggest to decrease diffusivities with a factor of 3 for the high salinity waters (Aberg) and to decrease the diffusivities by a factor of 10 for the low salinity waters (Beberg and Ceberg). This suggestions is, however, not clearly motivated. In contrast it seems more motivated to

- discard the increase in diffusivity due to the surface diffusion since the quantification of this effect is uncertain and implies improved retention properties,
- select the lowest diffusivity values (saline or fresh) to account for uncertainty in water chemistry,
- and to divide all diffusivities by a factor of 10 to account for uncertainty in spatial variability of porosity.

The analysis of Ohlson and Neretnieks builds on the porosity value of $5 \cdot 10^{-3}$ provided by Johansson *et al.* (1996). As discussed above this value is probably quite variable and my also be questioned for migration distances longer than the scale of laboratory diffusion experiments. However, in order not to double count the uncertainty ranges already derived for diffusivity, it is suggested to use $5 \cdot 10^{-3}$ for all cases. Furthermore, as previously discussed, for the low ionic strength waters of Beberg and Ceberg a 10 times smaller value, i.e. $5 \cdot 10^{-4}$ should be used for the anions Br, C, Cl, I in order to be consistent with the diffusivity adjustments.

Table 5.5.1 summarises the above suggestions.

Table 5.5.1: *Suggested quantification of uncertainties in matrix porosity and rock matrix diffusivities (D_e)*

Case	Aberg	Beberg	Ceberg
Matrix porosity			
All cases	$5 \cdot 10^{-3}$	$5 \cdot 10^{-4}$, for Br, C, Cl, I, $5 \cdot 10^{-3}$ for all others	$5 \cdot 10^{-4}$, for Br, C, Cl, I, $5 \cdot 10^{-3}$ for all others
Diffusivity			
Reasonable estimate	Saline in table A.2.5.2 (based on table 2 in Ohlsson and Neretnieks (1997), for high ionic strength).	Fresh in table A.2.5.2 (based on table 2 in Ohlsson and Neretnieks (1997), for low ionic strength).	Fresh in table A.2.5.2 (based on table 2 in Ohlsson and Neretnieks (1997), for low ionic strength).
Pessimistic	Pessimistic in table A.2.5.2 (surface diffusion increase is discarded, lowest values are selected regardless of water chemistry and all values are divided by 10)	Pessimistic in table A.2.5.2 (surface diffusion increase is discarded, lowest values are selected regardless of water chemistry and all values are divided by 10)	Pessimistic in table A.2.5.2 (surface diffusion increase is discarded, lowest values are selected regardless of water chemistry and all values are divided by 10)

5.6 Geosphere sorption

5.6.1 Source of information

Carbol and Engkvist (1997) provide sorption data in terms of K_d values by exploring different experimental databases, while considering the geology and water chemistry at the different sites. In addition, Bruno and Duro (1997) discuss uncertainties in these estimates.

5.6.2 Use in SR 97, modelling approach and conceptual model uncertainties

The far-field migration code FARF31 (see chapter 3) models sorption inside the rock matrix as a linear process through the use of distribution factors or K_d values. In the model, the concentration of the dissolved substance is (linear) proportional (by the K_d) to the concentration of the sorbed substance.

As discussed by Carbol and Engkvist (1997) sorption is used as a common term for many different processes including chemi-sorption, electrostatic adsorption (ion exchange) and physi-sorption. When substances sorb on mineral surfaces two or all three processes can contribute to the sorption and one process can convert to another. Sorption processes can also transform into precipitation reactions. Clearly, it is not evident that the different sorption processes can be described by a simple linear term. Carbol and Engkvist (1997) conclude that the sorption coefficient is specific to the system studied, but within limits it is independent of the original concentration of the dissolved substance. Although the radioactivity in the repository is high, the molar amounts are small and thus also the concentrations. Consequently, the K_d concept is a fair model as long as it is selected consistently with the water chemistry in question (see also discussion in Carbol and Engkvist, 1995).

5.6.3 Data uncertainties, correlations and dependencies on other parameters

Carbol and Engkvist (1997) discuss the following influences on the sorption data and their uncertainty:

- temperature,
- influence of groundwater chemistry,
- influence of organic matter,
- influence of solid composition,
- selection of proper experimental data.

Bruno and Duro (1997) have not found experimental sorption data for other temperatures than 25 °C. The impact of other temperatures is thus unknown.

Carbol and Engkvist (1997) handle the impact on water chemistry by selecting K_d values from experiments using groundwater compositions relevant for the reference waters (see 5.1) of SR 97. It is mainly the ionic strength, pH and redox that affect the K_d. High ionic strength waters (such as Aberg and saline Beberg) affect sorption of alkali and to some extent the alkali earth metals and Carbol and Engkvist thus supply K_d values both for saline and non-saline waters. For those elements which sorb by surface complexation, the pH is an essential parameter. However, Carbol and Engkvist (1997) suggest that the effect is significant only if pH decreases below 4, i.e. far from the reference waters and thus only provide K_d values valid for pH>7, which is a condition covered by all reference waters. Since all reference waters are reducing, Carbol and Engkvist do not directly discuss the impact of redox, but the K_d values provided are selected such that they only are relevant for Eh<-200 mV. This restriction still covers all reference waters, but additional K_d values need to be supplied if other scenarios would result in higher Eh.

Carbol and Engkvist only briefly discuss the possibility that organic compounds (complexing agents) would impact the sorption. They conclude that the influence of humics is of minor importance in deep groundwaters with an organic content of less than 10 mg/l. The DOC (Dissolved Organic Carbon) is 1 mg/l, 6 mg/l and 2 mg/l for Aberg, Beberg and Ceberg, respectively, and thus lies below 10 mg/l, which means that the influence of organics can be neglected.

The reference geology system considered is crystalline granitic rock. It is clear that even within the limitation of granitic crystalline rock there are large mineralogical variations between countries and sites. Bruno and Duro (1997) note that the solid composition may have important influences on the sorption of the different radionuclides studied and that the mineralogy of the fracture fillings, which is the first part of the rock to be exposed by the migrating water, may differ from the host rock. However, Carbol and Engkvist conclude that almost always the same highly sorbing minerals are present in the rock, although in different proportions. The water composition is of much greater importance than the rock composition.

The difference in experimental data bases arise mainly from differences in groundwater composition and the judgement by the authors. It has been suggested that there is a difference between data from intact and crushed rock materials, but Carbol and Engkvist do not give significance to this. In those cases for which a large number of experimental studies have been performed on a particular element and the results are scattered, the data selected concern similar groundwater systems or are reported from experimental groups that have produced data for other elements which show consistency regarding chemistry. Clearly, the final selection of data is based on the judgement of the authors. For some elements, like Sm, Eu, Ho and Cm there are very few (if any) data. Based on the similarity in chemistry with Am, Carbol and Engqvist suggest to use Am values for these elements. However, it turns out that they have reduced the K_d:s somewhat. The difference is, however, negligible and furthermore the elements are rare also in spent fuel. For consistency it thus suggested to stick to the values suggested by Carbol and Engqvist (1997).

Based on the above consideration Carbol and Engkvist provide *reasonable estimate* sorption values for ”saline” and ”non-saline” waters. In addition, they provide uncertainty intervals based on the scattering of experimental data found in the literature. Only values representative for conditions in Sweden (i.e. including Aberg, Beberg and Ceberg) have been included. The reported uncertainties thus appear to represent true ignorance rather than variability embedded in varying groundwater chemistry etc. The latter complications are already covered as discussed above. The interested reader may find arguments for the recommended values and ranges for each investigated element in Carbol and Engkvist. The data recommended are displayed in table 12-1 of their report and in table A.2.6.2 of appendix A.

In reviewing the data by Carbol and Engkvist (1997) Bruno and Duro (1997) only suggest minor modifications. In short they suggest to

- decrease recommended K_d value for Sr under saline conditions by a factor of 10,
- reduce the upper limit of K_d for Pa to 1 m^3/kg,
- reduce the recommended K_d value of Pu to 1 m^3/kg.

In addition, they sometimes question whether it is at all possible to produce uncertainty ranges. However, considering the judgmental nature of the *reasonable estimate* in the first place, the wide ranges in the uncertainty intervals suggested by Carbol and Engkvist (1997) and the relative insensitivity of retardation to K_d values it does not seem warranted to change the values suggested by Carbol and Engkvist (1997) for use in SR 97.

5.6.4 Quantification of uncertainties

Based on the arguments presented above, and in more detail by Carbol and Engkvist it appears evident that the *reasonable estimate* sorption coefficients to use in SR 97 should be taken from the reasonable estimate values as suggested by table 12-1 in Carbol and Engkvist. To be consistent with water chemistries (see 5.1) one should use ”saline” values for Aberg and ”non-saline” values for Beberg and Ceberg. Furthermore, for Te, U and Np reducing conditions should be assumed, i.e. the values for Tc(IV), U(IV) and Np(IV) since there is no experimental foundation to use the values for the oxidising conditions.

A clearly *pessimistic* selection of sorption coefficients is to select the lowest K_d values (for saline as this results in lower values) in table 12-1 of Carbol and Engkvist. Such a selection would cover both the experimental uncertainties and the uncertainty in water chemistry at the sites. However, for Ceberg it appears evident that non-saline conditions will prevail for the base case and initiallly defect canister scenario (see section 5.1). Consequently, the lowest fresh water values could be used for Ceberg.

Carbol and Engkvist supply ranges of values but do not discuss correlation between elements or potential forms of the distribution. Many of the potential influences causing correlation have already been ruled out (see previous section) leaving much of the uncertainty as an experimental uncertainty. There correlation between elements is less obvious.

The following approach is suggested. For Aberg one should apply the full range for saline water in Table 12-1 of Carbol and Engkvist assuming uniform distribution. For Beberg one should primarily apply the full range of non-saline waters in Table 12-1, but an alternative case with saline waters should be considered. For Ceberg one should apply the full range of non-saline waters in table 12-1. For all three sites one should consider to compare a case with no correlation between elements and a case with full correlation between elements. Table 5.6.1 summarises the suggestions.

Table 5.6.1: *Suggested quantification of uncertainties in rock K_d values*

Case	Aberg	Beberg	Ceberg
Reasonable estimate	Reasonable estimate reducing saline values in Table 12-1 in Carbol and Engkvist (1997). Use Tc(IV), U(IV) and Np(IV).	Reasonable estimate reducing non-saline values in Table 12-1 in Carbol and Engkvist (1997). Use Tc(IV), U(IV) and Np(IV).	Reasonable estimate reducing non-saline values in Table 12-1 in Carbol and Engkvist (1997). Use Tc(IV), U(IV) and Np(IV).
Pessimistic	Lowest value in range for saline in Table 12-1 in Carbol and Engkvist (1997).	Lowest value in range for saline in Table 12-1 in Carbol and Engkvist (1997).	Lowest value in range for fresh (reducing) in Table 12-1 in Carbol and Engkvist (1997).
Probabilistic cases	Apply full range for saline water in Table 12-1 assuming uniform distribution. Compare no and full correlation between elements.	Apply full range for non-saline water in Table 12-1 assuming uniform distribution. Compare with saline and full correlation between elements. Evaluate impact of saline water.	Apply full range for non-saline water in Table 12-1 assuming uniform distribution. Compare no and full correlation between elements.

6 Groundwater flow

Groundwater flow affects radionuclide release and migration in several ways, as is displayed in figure 6.1. It affects near field release, migration through the geosphere and the distribution of discharge into the biosphere. A hydrogeological model of a site requires input from a geological structure model and specific hydrogeologic data. For practical reasons the hydrogeologic models are divided into a regional model and a more detailed site scale model. This means that also the uncertainties involved in the transfer of boundary conditions between different size scale models needs to be addressed. This chapter discusses the rationale and uncertainties of the different hydrogeologic analyses conducted within SR 97. However, evaluation of the results of these analyses is primarily made when discussing hydrogeologic input to the geosphere migration (chapter 7) and to the biosphere modelling (chapter 8).

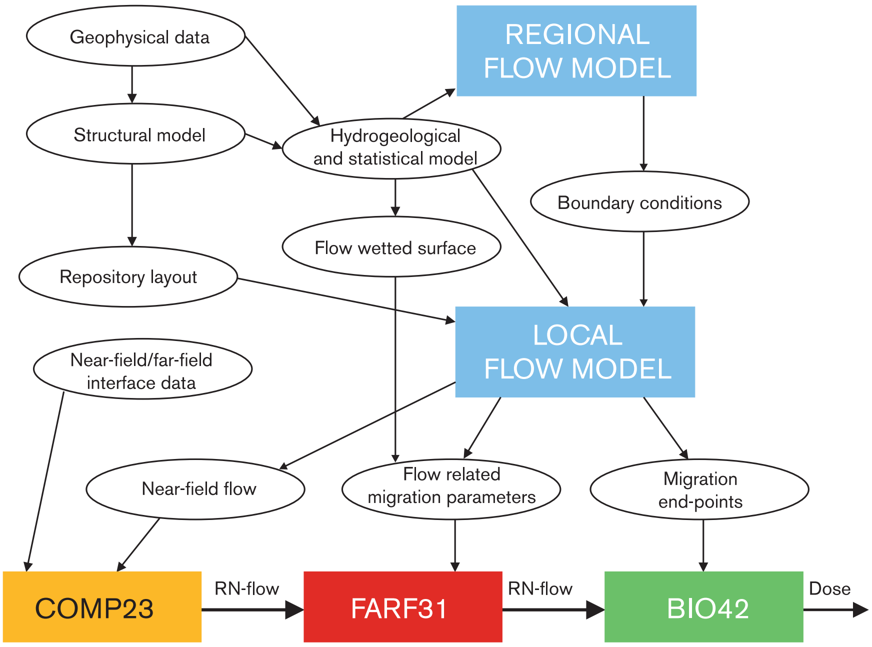


***Figure 6.1**: The different hydrogeologic analyses used to provide the hydrogeologic input to the main chain of consequence codes*

6.1 Geological Structure Models

6.1.1 Source of information

The geological structure models are descriptions of the location, geometry and geological properties of fracture zones at the given site. The Aberg model was established by Wikberg (ed, 1991) and updated by Rhén *et al.* (1997). The Beberg model is summarised by Alhbom *et al.* (1991). The Ceberg model has been updated by Hermanson *et al.* (1997), but Albino and Nilsson (1982) did much of the original interpretation. Saksa and Nummela (1998) evaluate uncertainties in these models.

The geological structure models are based on direct observations such as outcrop and core mapping and indirect data such as geophysical measurement. These data needs to be interpreted in the context of an interpretation model. The wealth of data varies between the sites as well as the approaches to interpretation.

6.1.2 Use in SR 97 and modelling approach

The geological structure model is used for repository layout and as input to the hydrogeological characterisation and mechanical characterisation of the different sites. For the layout both mechanical and hydrogeological properties of fracture zones are used as input. It is assumed that the zones have hydrogeological properties distinct from the remaining rock mass. The use of the structural data as input to the hydrogeological model is further discussed by Walker *et al.* (1997) and in section 6.3.

The conceptual model assumes that fracture zones have properties distinct from the other rock mass. The cornerstone of the fracture zone model is further that zones are planar and show a relatively uniform continuation along the strike and dip directions.

6.1.3 Data uncertainties, correlations and dependencies on other parameters

Saksa and Nummela (1998) state that uncertainty is a natural part of all geoscientific investigations. Uncertainties are related to *conceptualisation* related issues, errors in *data and interpretation*, and *sampling limitations* of the surveying techniques. The selection of geological concepts, structural geometry concepts and property concepts is judgmental and thus constitute an uncertainty. These uncertainties are related. There may be inconsistencies in the way the concepts have been applied. Errors in data and interpretation stem from the fact that many geophysical investigation methods are indirect and the interpretation models do not have unambiguous geometric or parametric solutions. Sampling limitations of the surveying techniques are introduced by many sources. A thick overburden does not allow outcrop mapping and masks surface geophysical measurements. The measurements do not cover the whole volume of interest, there will always remain rock volumes between boreholes. The sensitivity and detection capability in respect to the targets varies spatially in the volume studied and in a complicated way.

Saksa and Nummela (1998) consider these uncertainties when evaluating the proposed structure models of Aberg, Beberg and Ceberg. They compare, and assess by expert judgement, the applied concepts for each site. When possible they check original data, used methods and interpretations made. In addition they apply additional interpretation methods on the original data. In short they conclude the following:

- The models do not contain fractures and fracture zones in the scale from 10 to 300-1000 meters for Beberg and Ceberg, even though such fractures are judged to exist.

- No new structures proposed for the Aberg regional structure mode. The potential uncertainties are larger in the site scale, partly stemming from the fact that the region just outside Aberg (Äspö) is covered by sea and due to the complex geology of the site. Still *no new or altered structures* in the Aberg structural model are suggested.

- The Beberg structural model in the regional scale is considered less certain since additional interpretation techniques could have been applied. In the site scale additional uncertainty stems from a partly unclear conceptual model (rules for cut-off etc.) A great deal of data is also non-interpreted. *Six additional* lineaments to be considered as *structure variants* are suggested. Furthermore, one should note that the conceptual model used did not consider fracture zones in the size range 10 m - 1000 m, in contrast to Aberg where these sizes are partly considered.

- For the Ceberg regional scale model there is an uncertainty whether some fracture zones exists. In the site scale the conceptual model is clearly defined, but there are a number of non-interpreted fracture sections in some boreholes. There is also uncertainty that some diabase dikes cannot be detected by the used geophysical methods. Altogether *six structures* are proposed as *variants* to the original Ceberg geological structure model. Furthermore, one should note that the conceptual model used did not consider fracture zones in the size range 10 m - 1000 m, in contrast to Aberg where these sizes are partly considered.

Despite the fact that Saksa and Nummela (1998) only suggest alterations to the structure model for Beberg and Ceberg, they also claim that the total, but not quantifiable, uncertainty is largest at the Aberg site model, second largest at Beberg and lowest at Ceberg. For the Aberg site scale Saksa and Nummela (1998) state that the carefully investigated volume is quite small and the question could be asked whether this volume is representative of the site conditions in general. It has been suggested that the actually investigated volume is an anomalously fractured, tectonised unit of its own. It could thus be questioned if the high fracture density of Aberg also continues in the rest of the site scale volume.

6.1.4 Quantification of uncertainties

The *reasonable estimate* structure models for Aberg should be the one provided by Rhén *et al.* (1997), for Beberg the one in Anderson *et al.* (1991) and for Ceberg the one by Hermanson *et al.* (1997). The additional structures in Beberg and Ceberg suggested by Saksa and Nummela (1998) should rather be seen as *variant* interpretations and not as ”corrections”.

The effect of alternative structure models cannot be predicted a priori. This means that it is not possible to select a *pessimistic* structure model. The approach rather has to be to study the implications of alternative structure models in order to explore whether any of possible alternatives would lead to less favourable performance than the *reasonable estimate* structure model.

Table 6.1.1 summarises the above suggestions.

Table 6.1.1 *Suggested quantification of uncertainties in structure models*

Case	**Aberg**	**Beberg**	**Ceberg**
Reasonable estimate	Rhén *et al.* (1997)	Andersson *et al.* (1991)	Hermanson *et al.* (1997).
Pessimistic	Not applicable.	Not applicable.	Not applicable.
Variants	No variant	Additional structures as suggested by Saksa and Nummela (1998).	Additional structures as suggested by Saksa and Nummela (1998).

6.2 Repository layout

The repository layout may be taken as a fixed input to the assessment calculations and should thus formally not be addressed in a document of this kind. On the other hand the repository layout is determined from the structure model information and the repository layout affects the parameter selection in subsequent analysis. For this reason also repository layout is discussed here.

Source of information

The SR 97 repository layout is developed by Munier *et al.* (1997). They use the structure models (see 6.1) as input to locate a repository at the respective sites using the following rules.

Use in SR 97

The repository layout is used to find out positions from which to determine near-field flow and near-field chemistry and to find starting positions for far-field migration. Indirectly the repository layout also affects the selection of model domains for the detailed hydrogeological models. However, from the strict safety assessment point of view the repository layout is regarded as fixed - and the analyses should explore the consequences of this layout.

Uncertainties in relation to repository layout

Uncertainty in structure model should certainly be reflected in some flexibility in the repository layout. Obviously, one would not place deposition holes in major zones. On the other hand it would not be correct to always adopt the repository layout to every variant of structure models. In reality, the precise locations of fracture zones are not known. The repository layout should thus, within limits, be fixed for different variants. Clearly the proper procedure for developing a repository layout would be to first develop the structure models with uncertainties and then suggest repository layouts that reflects these uncertainties. One could, however, note that the layout principles partly are introduced in order to account for uncertainties in structure model. Consequently, for the SR 97 application there is no uncertainty in repository layout. The implications of uncertainty in structure models are to be explored by considering variants of structure models for the same repository layout.

Recommended approach

For SR 97 the repository layouts as suggested by Munier *et al.* (1997) will be taken as fixed. However, for Aberg Munier *et al.* (1997), suggest alternative layouts. Of these the layout ”optimised after the rock block form” (figures 6-14 and 6-15) should be used in the analysis since it concerns a region of Aberg where the knowledge of the structures is much better than in the regions of other suggested layouts.

Table 6.2.1summarises the above suggestions.

Table 6.2.1 *Suggested handling of repository layout*

Case	Aberg	Beberg	Ceberg
Fixed	As suggested by Munier *et al.* (1997), fig 6-14 and 6-15.	As suggested by Munier *et al.* (1997).	As suggested by Munier *et al.* (1997).

6.3 Hydrogeological model: Data and geostatistical models

6.3.1 Source of information

Walker *et al*. (1997) compile existing data and descriptions for use in the hydrogeologic modelling of the Aberg, Beberg and Ceberg sites. They provide modelling teams with parameter values for inputs to numerical flow models on the regional and site scales. Uncertainties are discussed and some variants to the suggested estimates are presented.

The information compiled is taken from several key sources, including the SKB SICADA database, the Swedish Geological Survey (SGU) well database, the SKB Geographic Information System (GIS), the Swedish Land Survey (LMV) databases, and published SKB reports. These sources contain information on boreholes, single borehole tests, interference tests, tracer tests, geophysics and tunnels observation. The geological structure models, in particular, are based on the reports by Rhén *et al*. (1997)

(for Aberg), Andersson *et al*. (1991) (for Beberg) and Hermanson *et al*. (1997) (for Ceberg) as already discussed in section 6.1.

When comparing the sites it is important to note that the site characterisation programme at each site were quite different. Aberg has the most extensive database and is the only site where there also are measurement from a tunnel at the site. Ceberg, in comparison, is the site with least amount of data. More detailed information on data sources for the different sites are available in Walker *et al*. (1997).

6.3.2 Use in SR 97, modelling approach and conceptual model uncertainties

The hydrogeologic models provided are mainly used as input to regional hydrogeological models and to detailed scale stochastic continuum hydrogeological models (see sections 6.4 and 6.5 below). The underlying conceptual model of the rock assumed is one of a *rock domain* described as a spatially varying but still continuous porous medium intersected by *conductor domains* (fracture zones), also modelled as porous media, but of hydraulic properties distinct from the rock domain. The approach further assumes a nested approach using a *site scale* (1 - 6 km^2) model, with relatively much detail in conductive structures, embedded in a *regional scale* (100 - 200 km^2) model with less geometrical detail, but large enough to include the regional flow system.

It is well established that the main driving force for groundwater flow is gravity, which through topographical differences will result in a distribution of re- and discharge areas. Inertial effects can be neglected. There are possibilities for coupled phenomena such as hydro-mechanical couplings, thermal buoyancy, density effects due to salinity and concentration differences as well as clogging or weathering of migration paths.

Density variations due to the heat production from the waste are fairly limited. In cases where the natural hydraulic gradient is significant, which usually is the case, Thunvik and Braester (1980) show that the thermally induced driving force can be neglected. However, the heat driving force may need to be considered when there are no other driving forces, which could be the case for a very deep repository in saline water (Claesson and Probert, 1996).

Modelling of hydro-mechanical couplings is of a research character for example within the framework of the international DECOVALEX-project (see e.g. Stephansson *et al*. 1996). Hydromechanical effects may be important in the vicinity of tunnels and may need to be considered for extreme events during glaciations. However, in most of the rock mass the added affect of hydromechanical changes, is probably minor, at least before a glaciation event.

Large density variations, for example due to highly saline waters, need to be incorporated, at least in large scale modelling. When considering density dependent flow it is usually not sufficient to assume steady-state flow (see e.g. Voss and Andersson, 1993). Both Aberg and Beberg show significant levels of salinity at depth as is also discussed by Walker *et al*. (1997). The need to incorporate varying salinity for

Aberg and Beberg is acknowledged in the regional groundwater flow analysis in SR 97 (see Svensson, 1997a, Hartley *et al.*, 1998 and section 6.4), but only the Beberg analyses combine this with changing boundary conditions. For practical reasons, varying density or varying boundary conditions are not included in the site scale analyses. The implications of this for the site scale analyses is further discussed in section 6.4 (and section 6.5).

Salinity and temperature also affect the hydraulic conductivity. This means that the conductance of the rock should rather be discussed in terms of permeability than hydraulic conductivity (see e.g. Bear, 1976), but in practice the influence is rather small.

The geometrical description of the conduits in the rock is one important conceptual uncertainty regarding hydrogeological models of crystalline rock. There exists conceptually different structure models, such as homogeneous porous medium, stochastic continuum, discrete fracture network and channel networks.

- In the stochastic continuum (SC) approach (e.g. Matheron, 1973 or Neuman, 1987 followed by many others) it is assumed that the permeable features of the rock mass may be described as a continuous, but spatially varying hydraulic conductivity field. Conceived advantages of the stochastic continuum concept are that the models can be applied to relatively large regions, that they, through multiple realisations, provide a means to handle uncertainty and spatial variability and that the models can be conditioned on point data. However, there are also question marks regarding their applicability. Key properties of a stochastic continuum model are the underlying statistical distribution and the associated model of spatial correlation, which will determine the effective connectivity of modelled rock mass. Different stochastic models exist (Gómez-Hernández and Srivastava, 1990), for example parametric, non-parametric, and fractal. There is little direct experimental evidence to support any particular correlation structure. In addition, simulation results (e.g. Tsang *et al.*, 1996) also show that the flow distribution and the migration paths strongly depend on the model actually selected.

- In the discrete fracture network (DFN) approach a network of discrete fractures (usually discs) of different size, orientations, locations, and hydraulic properties represents the rock mass. All these properties are regarded as stochastic parameters. One of the conceived advantages of the DFN models are that they actually try to describe flow as it can be observed from individual bore holes and tunnels and thus lend itself to a co-ordinated interpretation of structure and hydraulic data. Another potential benefit for transport applications is that they have the intuitive benefit of actually describing the interaction between flow and the rock itself, and can thus provide direct estimates of the correlation between flow and the retention parameters. On the other hand discrete network models are difficult to apply in the large scale and also depend on parameters that may be very difficult to estimate in these large scales.

- Another alternative for the detailed hydrogeological (and transport) modelling is the Channel Network concept (see e.g. Gylling *et al.*, 1994 or Moreno *et al.*, 1997). In the channel network model flow and transport takes place in a network of one-

- dimensional channels. The model is characterised by the conductivity distribution of the channels, transport properties and frequency of channels. However, in contrast to the discrete fracture network concepts the channel network models do not use structural information explicitly. One could argue that conceptually the channel network model is quite similar to an integrated finite difference model, but where the explicit channels facilitate particle-tracking algorithms. As with both the stochastic continuum and the discrete network approach the migration path characteristics will depend on the effective connectivity (i.e. a function of channel permeability and frequency distribution).

In conclusion, it appears evident that for source term analyses and radionculide migration it is necessary to represent the pronounced spatial variability at the scale of the source term (i.e. the deposition holes). There is also a need to represent uncertainty with a stochastic continuum approach and at least discuss the applicability of different conceptual models. For this reason SR 97 also includes an evaluation of the detailed scale hydrogeology using discrete network and channel network models as further discussed in section 6.5 below. Due to the conceptual differences between the models Walker *et al*. (1997) can only partially fulfil the need for input data to these models.

6.3.3 Data uncertainties, correlation and dependencies on other parameters

For the regional scale, Walker *et al. (*1997) generally base hydraulic conductivity estimates of the *rock domain* on SGU data, but with depth zones from on-site packer tests. Regional lineaments are treated as *conductive domains*, but with hydraulic properties inferred from site scale packer tests. The geometry of the conductive domains in the site scale are taken from the site structure models (see 6.1). The statistical distributions of the *rock domain* hydraulic conductivity and the *conductor domain* hydraulic conductivity are estimated from on-site packer test data from these respective domains. Top surface boundary conditions are obtained from evaluation of surface hydrology. At least the following uncertainties can be associated with this approach:

- uncertainty in surface hydrology,
- selection of rock and conductor domains,
- interpretation and availability of hydraulic tests (density of data and data below the measuring limit),
- scaling and correlation structure,
- potential depth dependence of hydraulic conductivity,
- potential correlation between rock type and hydraulic conductivity,
- potential anisotropy of hydraulic conductivity.

These uncertainties are discussed in the following.

Surface hydrology

Walker *et al.* (1997) discuss the surface hydrology, groundwater table and distribution of recharge discharge areas at the respective sites. In general, recharge will occur in elevated regions and flow to discharge areas at lower elevations. The details of the surface hydrology could be quite complex. The groundwater table does not fully follow topography and discharge/recharge is difficult to measure with high accuracy. Existing information on precipitation, topography and surface hydrology still make qualitative comparisons between models and reality possible. This means that the top boundary condition is subject to uncertainty and needs to be addressed by the hydrogeological modelling. This issue needs to be handled in the regional scale modelling and is further discussed in section 6.4.

Selection of rock and conductor domains

There are uncertainties connected to the selection and property assignment of rock and conductor domains. Regional lineaments are in reality one-dimensional features inferred to be the topographic extension of a bedrock feature. The approach taken is that it is anticipated that some of the well-expressed lineaments might be modelled as conductive fractured zones with parameter values assigned by expert judgement and extrapolation of the few measurements available (for details see Walker *et al.*, 1997). In the site scale it is assumed that the fracture zones in the structure model (see section 6.1) represent the conductor domain. In the site scale these zones have usually been tested hydraulically. Still the nature, width and extent of a regional conductor domain should be considered uncertain and there is also uncertainty in the site scale conductor domains. In order to handle this uncertainty Walker *et al. (*1997) suggest an alternative (hypothetical) variant for Beberg with a deep subhorizontal zone and an alternative interpretation of Ceberg based on Askling (1997). However, it seems more appropriate to instead consider the variants suggested by Saksa and Nummela (1998) as they base their suggestions on an assessment of the currently available information. This will be further discussed in section 6.5.

Hydraulic conductivity estimates

The hydraulic conductivity estimates are based on various interpretations of packer tests and well tests. The tests at the different sites are of dramatically different duration, which may lead to different volumes being tested and consequent bias. The assumptions involved in the interpretation of the test also imply uncertainty. Walker *et al.* (1997) note that the uncertainty in such interpretation may be one order of magnitude (Geier *et al.*, 1996), but do not further evaluate whether the interpretations of the A- Be- or Ceberg estimates are subject to such biases. A connected problem is the amount of data censored by the measuring limit. The problem is most severe at Ceberg where 36% of all injection tests lie below the measuring limit. Partially this is due to the low permeability of the rock mass, but the measurement technique used at Ceberg is less sensitive than methods used in more recent site investigations. Walker *et al.* (1997) attempt to correct the statistical distributions for data below the measurement limit in order not to overestimate the mean and underestimate the variance, but note that there are difficulties associated with such corrections, in particular when data are spatially correlated.

The multiple scale variability of the rock, the mixed scale of hydraulic measurements, the nested modelling approach and the use of variable size blocks in the numerical models poses a problem on which ”equivalent” permeability value to assign to model blocks of sizes larger than the measuring scale. Scaling rules can be derived under a number of restrictive assumptions, but given the high variability in measured permeability and the fracture nature itself it is not evident that such rules apply to crystalline basement rock. Walker *et al.* (1997) suggest a scaling rule, at all sites, using a relation based on a regression analysis of different size hydraulic tests at Äspö (Rhén *et al.,* 1997). They do acknowledge that this approach builds one a series of non-proven assumptions and that there are no similar data from Beberg or Ceberg, but the approach is chosen, as there is little other information to apply. The suggested application of the scaling rule differs somewhat between the regional scale and the site scale as explained in the following.

In the regional scale it is suggested to use the regression values as a starting value, but then to calibrate these values by comparing calculated and measured regional head distributions and the patterns of recharge and discharge. However, given the uncertainty in surface hydrology, especially quantification of recharge/discharge, such a calibration could be questioned. Furthermore, any scaling rule implies approximations and it should be further evaluated which aspect of the regional flow that needs to be preserved. Clearly, for performance assessment the regional flow affects the analysis through the boundary conditions applied to the site scale models. This implies that the uncertainty in regional scale ”equivalent” hydraulic conductivity needs to be addressed when discussing uncertainty in boundary condition transfer between regional scale and site scale models (see Follin, 1999 and section 6.4).

In the site scale, which require geostatistical parameters, the correlation structure is only calculated along boreholes (i.e. where there is data) and is furthermore up-scaled to suite the block size of the computer model using the code INFERENS (Geier, 1993ab). Walker *et al.* (1997) suggest to apply the Äspö regression relationships to determine a preliminary value of the geometric mean, but to calibrate this value such that the site scale models reproduce fluxes calculated by the regional models. (This procedure has, however, not been adopted within the subsequent modelling, see section 6.5). The approach has the benefit of making the flow consistent in the site and regional scale models. However, the questions about scale, and the lack of field data to determine correlation structure are significant for hydrogeological modelling as these assumptions determine both flow and flow distribution as shown e.g. by Tsang *et al.* (1996). The lack of data to support one of the main characteristics of the stochastic continuum models is a main reason to also apply alternative models for the detailed scale (see section 6.5). As a variant Rhén *et al*. (1997) attempt to correlate hydraulic properties to different rock domains for Aberg. The correlation is quite weak but it is still suggested as the base case by Walker *et al*. (1997). Division into different rock domain types is not suggested for the other two sites.

The measured hydraulic conductivities tend to decrease with depth. Previous assessments (e.g. SKBF, 1983) attempted to describe this decrease with regression curves. However, inspection of the data shows little rationale for these curves. Instead Walker *et al. (*1997) divide the data into a few depth zone classes, both for the regional and the site scale. Within each depth zone there is little evidence for further depth dependence. There is comparatively little data to show the depth dependence of hydraulic conductivity of the conductor domains. In general, the standard assumption by Walker *et al. (*1997) is to adopt the same depth zones in the conductor domains as the ones used in the rock domains, but alternatives with different depth zones are also presented.

Rhén *et al.* (1997) suggest that the (regional rock domain) hydraulic conductivity of Aberg could be anisotropic in the direction of regional stress and also suggest a variant to analyse the importance of this. For this reason Walker *et al.* (1997) also suggest variants with such an anisotropy for Beberg and Ceberg even if there are no measurements available to confirm (or reject) such assumptions. Qualitatively, such a variant could find support from observed preferential directions of the fracturing as the Schmidt nets roughly agree with the direction of regional stress.

Tables 6.3.1ab display resulting hydrological geostatistical properties of the sites. One need to consider all the non-quantified uncertainties discussed above before exploring the differences between sites. Still the table suggests that Ceberg has hydraulic conductivity two order of magnitude less than the other sites and a much less pronounced difference between fracture zones and rock mass.

Table 6.3.1a *Geostatistical properties for site scale of rock domains at - 500 m of the three sites as estimated by Walker et al., 1997 (source table indicated) assuming exponential variograms.*

Site	*$\log_{10}(K)$ (m/s)*	*Total Variance*	*Range (m)*	*Scale (m)*	*Table in Walker et al. (1997)*
Aberg	-8.5	2.72	97	24	A-5
Beberg	-7.9	0.77	188	24	B-5
Ceberg	-10.3	1.15	57	25	C-5

Table 6.3.1b *Upscaled conductor domain properties, for site scale, suggested by Walker et al. (1997).*

Site	*Range $\log_{10}(K)$ (m/s)*	*Scale (m)*	*Table in Walker et al. (1997)*
Aberg	-8.2 to -5.3	24	2-9
Beberg	-7.7 to - 4.8	24	3-6
Ceberg	-9.7	25	4-5

As can be seen from the discussion Walker *et al.* (1997) suggest to handle part of the uncertainties as discussed above through variants. Tables 6.3.2ab summarise their suggestions.

Table 6.3.2a: *Variants in regional scale hydrogeological models as suggested by Walker et al (1997).*

Variant description	**Aberg – Table 2-10 in Walker *et al.* (1997)**	**Beberg – Table 3-7 in Walker *et al.* (1997)**	**Ceberg - Table 4-6 in Walker *et al.* (1997)**
Rock domain			
Base case	Scaled from on-site packer test data. Depth zones	Scaled from on-site packer test data. Depth zones	Scaled from on-site packer test data. Depth zones
Correlation with rock type	Yes	not suggested	not suggested
Anisotropy	In direction of maximum horizontal rock stress.	In direction of maximum horizontal rock stress	In direction of maximum horizontal rock stress
Conductor domain			
Base case	Regional lineaments of Rhén *et al.* (1997). Depth zones as for base case rock	Mapped lineaments. Hydraulic conductivity inferred from packer tests. No depth zones	Mapped lineaments. Hydraulic conductivity inferred from packer tests. Depth zones.
Alternative depth zones	No depth zones	Depth zones	not suggested
Alternative lineaments	not suggested	Hypothetical sub-horizontal fracture.	Alternative interpretation based on Askling (1997)

Table 6.3.2b: *Variants in site scale hydrogeological models as suggested by Walker et al. (1997).*

Description	**Aberg – Table 2-10 in Walker *et al.* (1997)**	**Beberg -Table 3-7 in Walker *et al.* (1997)**	**Ceberg - Table 4-6 in Walker *et al.* (1997)**
Rock domain			
Base case	Upscaled from packer tests assigned to 5 different regions/rock types	Upscaled from packer test, with depth zones.	From packer test, with depth zones
Anisotropy	In direction of maximum horizontal stress	In direction of maximum horizontal rock stress.	In direction of maximum horizontal rock stress.
Conductor domain			
Base case	Fracture zones with properties inferred from interference tests and spinner tests	Fracture zones as in SKB91 no depth zones. Inferred from packer tests	Fracture zones of Hermanson *et al.* (1997), properties and depth zones from packer test data. Uniform for all zones.
Depth zones	not suggested	Depth zones same as for rock domain.	not suggested.
Alternative fracture zones	In accordance with alternative in Rhén *et al.* (1997)	Hypothetical sub-horizontal fracture zone	Three variants with additional zones.

6.3.4 Quantification of uncertainties

The base case parameters suggested by Walker *et al.* (1997) are based on a multitude of data, which to the extent possible have been evaluated consistently. There has been a strive to base necessary assumptions on observations. Consequently, the base case suggested must be regarded as *reasonable estimate* hydrogeological models of the three sites.

It is not possible to define a *pessimistic* case of a hydrogeological model as the impact on performance is quite complex (see figure 6.1). A pessimistic case can only be selected when analysing output from different hydrogeological models, i.e. in the selection of input parameters to the consequence analysis. Such pessimistic selections are discussed in chapter 7 (near-field and far-field) and chapter 8 (biosphere).

The discussion of *uncertainties* show that both conceptualisation and parameterisation of hydrological models is quite uncertain, even if part of this uncertainty may be of little impact for repository performance. The *variants* suggest by Walker *et al*. (1997) explores some of this uncertainty, but possibly not all. Evidently the structural variants suggested by Saksa and Nummela (1998) need to be considered. The alternative conceptual descriptions given by a discrete network representation or by a channel network representation need also be considered. Additional uncertainties may be introduced in the transfer of boundary conditions from the regional scale analysis to the site scale analysis.

The handling of all of the above these possibilities will be discussed in section 6.5. Table 6.3.3 summarises the above suggestions. However, it should be noted that there is other information to consider in the selection of which variants to finally evaluate. This will be discussed in subsequent sections. Section 6.5 describes which variants were actually analysed within SR 97.

Table 6.3.3 *Suggested quantification of uncertainties in hydrogeological models. Table 6.5.1 describes variants actually analysed within SR 97.*

Case	Aberg	Beberg	Ceberg
Reasonable estimate	Base case as displayed in table 6.3.1	Base case as displayed in table 6.3.1	Base case as displayed in table 6.3.1
Variants (for final selection see section 6.5)	Discuss or evaluate variants as suggested by Walker *et al.*, 1997 (see table 6.3.1). In addition uncertainty in boundary conditions to site scale models (see discussion in 6.4) Consider DFN and Channel Network models.	Discuss or evaluate variants as suggested by Walker *et al.*, 1997 (see table 6.3.1). New structures suggested by Saksa and Nummela (1998) In addition uncertainty in boundary conditions to site scale models (see discussion in 6.4) Consider DFN and Channel Network models.	Discuss or evaluate variants as suggested by Walker *et al., 1997* (see table 6.3.1). New structures suggested by Saksa and Nummela (1998) In addition uncertainty in boundary conditions to site scale models (see discussion in 6.4) Consider DFN and Channel Network models.

6.4 Regional models and boundary conditions for detailed scale hydrogeological analyses

This section discusses the regional scale analyses made for providing boundary conditions to the repository scale analysis

6.4.1 Source of information

Svensson (1997a), Hartley *et al.* (1998) and Boghammar *et al.* (1997) perform the regional groundwater modelling of Aberg, Beberg and Ceberg respectively. The modelling essentially builds on the hydrogeologic data compiled by Walker *et al.* (1997). Follin (1999) evaluates the uncertainties in this modelling with special attention to the description of the hydrogeologic processes and boundary settings.

6.4.2 Use in SR 97, modelling approach and conceptual model uncertainties

The regional scale models are primarily used for setting boundary conditions to the site scale groundwater models and thus only indirectly provide data to the consequence analysis. As already discussed in section 6.3 the regional scale models are based on a non-stochastic porous medium approach, where the rock is assumed to consist of *rock domains* intersected by *conductor domains* (fracture zones), both modelled as porous media, but with different hydraulic properties in the respective domains. At Aberg Svensson (1997a) considers steady state flow with and without the effect of varying density from the salinity distribution. At Beberg Hartley *et al.* (1998) consider transient density (and non-density) dependent flow. At Ceberg Boghammar *et al.* (1997) consider steady-state constant density (non-saline) flow.

The conceptual model uncertainties connected to porous medium hydrogeologic modelling have already been discussed in section 6.3.2. In addition, the nested approach raises questions regarding the proper formulation of boundary conditions at the site scale model boundaries.

6.4.3 Data uncertainties, correlations and dependencies on other parameters

Follin (1999) discusses the following potential origins of the data uncertainties in the regional scale models:

- transfer of boundary conditions from regional scale to site scale,
- permeability distribution in regional models,
- density variations and shore level displacements,

- model domain size,
- lateral and top boundary conditions.

When evaluating the significance of these uncertainties, it is necessary to do this in relation to their effect on the boundary conditions to the site scale models. This means that it may be allowable to greatly simplify the hydrogeological description on the regional scale, provided the net effect on the boundary conditions is small.

Transfer of boundary conditions from regional scale to site scale

The standard procedure for transferring boundary conditions from the regional scale models to the site scale is to apply a prescribed pressure boundary condition on the site scale model taken from the pressure solution of the regional model at the locations of the site scale model boundaries. Follin (1999) points out that the boundary of the site scale models are not placed at real physical boundaries. This means that a pressure distribution along this boundary would change with changes of e.g. the hydraulic conductivity field in the site scale model, and the approach of using fixed pressure boundary conditions from the regional scale models is thus in principle incorrect. If the head values are used as artificial boundaries on the smaller domain, then the equivalent conductivity of the smaller domain must equal that of the corresponding portion of the regional model.

Clearly, the ultimate solution would be to extend the size of the simulation domain of the site scale models such that it coincides with more natural boundaries, but this is not practical. In future assessments Follin (1999) suggests the following procedure:

- generate the conductivity field on a scale of support that meets the site scale model (i.e. the scale of interest),
- aggregate the generated conductivities to blocks which coincide with the scale of support of the regional hydrogeologic model,
- solve the regional model problem and use the head solution as boundary condition for solving the site-scale hydrogeologic problem.

This procedure was not adopted within the SR 97 hydrogeological analyses. However, in order to check the magnitude of the potential error, Walker and Gylling (1998) checked the flows in the regional model and over the site scale model. For the base case of Aberg (see section 6.5) they found that the boundary fluxes deviated a factor of 0.5 (with higher fluxes in the regional model). It is possible that the hydraulic conductivities of the regional model could have been adjusted to make the flows even more equal, but also the small deviation found is in fact quite re-assuring considering other potential sources of errors. The problem nevertheless warrants the analyses of different boundary condition variants for the site scale analysis. This has also been considered in SR 97 (see section 6.5).

Permeability distribution

Walker *et al.* (1997) provide estimates of the regional scale permeability distribution at the sites. As discussed above (6.3), the uncertainty in these estimates, as well as the uncertainty in the structure models, are handled by formulating variants. Follin does not further discuss this. The action taken within SR 97 (see section 6.5) is to apply boundary conditions for the site scale model taken from a regional scale model with conductivities upscaled from the distribution used in the site scale model.

Varying density and shore level displacements

Dramatic alterations of boundary conditions to the regional groundwater model lies outside the scope of the base and initial canister defect scenarios. However, the ongoing shore displacement and its effect on the density stratification due to varying salinity in coastal areas, potentially needs to be considered.

Svensson (1997a) considers the density effect of salinity but not the ongoing shore displacement at Aberg. He also presents a variant without density stratification. At depths below 1000 m these variants differ significantly, with essentially no flow for the density variant, but at the proposed repository levels the differences are far less even if the flow is lower for the density case. Based on the general findings of Voss and Andersson (1993), Follin (1999) points out that the on-going shore level displacement, which can continue during the next 10 000 years, makes it questionable if the flow can be modelled as steady-state at Aberg. However, it may be possible to explore the significance of this potential limitation by comparing different boundary conditions variants based on the different regional scale variants (see section 6.5).

Hartley *et al.* (1998) consider the density effect of salinity and the changing boundary conditions at Beberg. A variant case with a different salinity boundary condition at the up-stream boundary showed little effect. Comparison between cases with and without density stratification indicates that the density effects for the Beberg setting tend to make some flow paths longer and deeper. Comparing cases with and without landrise show very small differences. However, the authors note that this is due to the fact that Beberg is quite far from the present shoreline. For a site close to the shoreline, such as Aberg, the effect is significant.

Even if there is a density dependent regional scale solution, Follin (1999) points out that it is not straight forward to use this solution as boundary conditions to a site scale model which does not consider density dependent flow. In this case there is no potential field which can be used to derive the velocity field. If the density stratification is mainly vertical, the vertical flow is proportional to the gradient of the “environmental head” (Davis and Da Wiest, 1996, p. 237-241) whereas the horizontal flow is proportional to the fresh-water head solution. Using fresh-water head also in the vertical direction would tend to exaggerate the flow. These difficulties should be explored by boundary conditions variants to the site scale models.

Boghammar *et al.* (1997) do not consider varying salinity or the ongoing shore displacement at Ceberg . This is probably not a major deficiency since the Ceberg groundwater is essentially fresh even if a very low salinity has been encountered at depth (Ahlbom *et al.*, 1991) and as the site is located far from the sea.

Model domain size

Follin (1999) points out that the Aberg model domain is not adapted to known or interpreted geological structures or water divides. Clearly, the domain chosen is non-optimal, but the impact on site scale boundary conditions may still be limited.

At Beberg the regional model domain is based on the structural evidence and also coincides with the regional domain considered by Saksa and Nummela (1998). However, Follin (1999) points out that the model domain is too small to capture all of the discharge even under present day conditions. This may make the simulation results sensitive to the downstream boundary condition. However, the impact is judged to be of second order and has not been further analysed within SR 97.

Also at Ceberg the model domain is based on the structural evidence and also coincides with the regional domain considered by Saksa and Nummela (1998). Follin (1999) also notes that the analyses by Boghammar *et al.* (1997) suggest that a smaller domain size is sufficient.

Top boundary conditions

The top boundary condition is subject to uncertainty and needs to be addressed by the hydrogeological modelling. The hydrologic top boundary condition at Aberg is defined as specified infiltration over the terrestial parts of the domain in combination with specified pressure over the marine parts. This setting implies no terrestial discharge of deep groundwater at any location above sea level. At Beberg, the top boundary is set as specified head to mimic present day groundwater table. At Ceberg different top boundary conditions were tried ranging from specified head, specified infiltration and head dependent flux. However, Boghammar *et al.* (1997) note that these different options gave rather similar results. The uncertainties generated by uncertainty in top-boundary conditions appear to be moderate.

6.4.4 Quantification of uncertainties

Despite some of the criticisms by Follin (1999) it still seems warranted to use the regional scale hydrogeologic model as *reasonable estimate* specified head boundary conditions to the site scale modelling. In addition, it appears worthwhile to explore the significance of the boundary conditions in some *variants*. Table 6.4.1 summarises the above suggestions. There may also be room for modelling development outside the scope of SR 97. These model developments are not anticipated to result in dramatically new modelling results, but are still motivated since they would alleviate the need for some of the reasoning now needed in order to motivate modelling choices.

Table 6.4.1 *Suggested quantification of uncertainties in regional models for boundary conditions in the site scale modelling. Table 6.5.1 defines which cases were actually analysed in SR 97.*

Case	Aberg	Beberg	Ceberg
Reasonable estimate	Use base case, transfer B.C. as specified head. Select hydraulic conductivity case consistent with site scale selection. Measure potential flux inconsistency between regional and site scale models.	Use base case, transfer B.C. as specified head. Select hydraulic conductivity case consistent with site scale selection. Measure potential flux inconsistency between regional and site scale models.	Use base case, transfer B.C. as specified head. Select hydraulic conductivity case consistent with site scale selection. Measure potential flux inconsistency between regional and site scale models.
Variants	Explore different variants of BC in order to explore impact of transient - density stratification	Discuss impact of transient density stratification	No need for further variants.
For development beyond SR 97	Consider scheme for nested modelling suggested by Follin (1999).	Consider scheme for nested modelling suggested by Follin (1999).	Consider scheme for nested modelling suggested by Follin (1999).

6.5 Hydrogeology in the detailed scale

6.5.1 Source of information

Walker and Gylling (1998), Gylling et al. (1999a) and Walker and Gylling (1999) describe the main alternative, i.e. the stochastic continuum model, for detailed scale groundwater flow modelling used in SR 97. The input data to this modelling is primarily taken from Walker *et al.* (1997) (see section 6.3) and with boundary conditions taken from the regional scale analyses (see section 6.4). However, Walker and Gylling (1998), Gylling et al. (1999a) and Walker and Gylling (1999) also re-evaluate the primary information in these sources, resulting in the formation of new variants and also discuss in detail the different uncertainties addressed by forming these variants

For Aberg there is also some alternative modelling exercises conducted both outside as well as within the framework of SR 97. This additional information is discussed in section 6.5.4. Due to its limits in scope this alternative modelling is not seen in SR 97 as full alternatives to the stochastic continuum analyses, but in a qualitative sense the results are useful in motivating flow related migration parameters (see chapter 7).

6.5.2 Use in SR 97, modelling approach and conceptual model uncertainties

Walker and Gylling (1998), Gylling et al. (1999a) and Walker and Gylling (1999) apply the stochastic continuum code HYDRASTAR (Norman, 1992). The flow solution is used as input to the assessment codes COMP23, FARF31 and BIO42, as will be further discussed in chapters 7 and 8.

The conceptual model uncertainty associated with groundwater flow modelling in crystalline rock has already been discussed in section 6.3.2. Some of these uncertainties are handled by formulating different variants of the stochastic continuum model, as will be further discussed in the next section.

6.5.3 Data uncertainties, correlation and dependencies on other parameters - HYDRASTAR

Based on the previous evaluations on structure models, hydrogeologic data and boundary conditions from the regional scale modelling, Walker and Gylling (1998), Gylling et al. (1999a) and Walker and Gylling (1999) suggest a base case for each site and some different *variants* of the repository scale HYDRSTAR hydrogeologic models. These suggestions were formed in discussions within a working group by considering the following set of parameters/conditions:

- domain size and location,
- boundary conditions (source of boundary conditions, type of boundary conditions, flux consistency),
- hydraulic conductivity model (scaling rule, geostatistical model, hydraulic units, EDZ, Backfill),
- flux consistency.

The exact definitions of the base cases and the variants are provided in Walker and Gylling (1998), Gylling et al. (1999a) and Walker and Gylling (1999).

Location and size of domain

The location and size of the simulation domain is usually determined by means of particle tracking in the regional scale groundwater flow model such that the suggested domain captures the main discharge locations. Walker and Gylling (1998), Gylling et al. (1999a) and Walker and Gylling (1999) show that this criterion is met for almost all variants of Aberg and Ceberg. In contrast, for some Beberg variants (variants 1 and 3, see below) most pathlines discharge through the bottom of the model and also through some of the vertical sides. For practical reasons, larger domain size have not been possible at Beberg, instead it is conservatively assumed that there is no further retardation along the pathlines discharging through any of the boundaries (the difference between pathlines discharging through different boundaries is shown in section 7.3, where far-field migration is discussed). With this (conservative) restriction it appears that the domain size used is sufficient.

The model discretisation should preferably be as small as the support scale in the measurements, but large enough to be practical for available computer resources. For Aberg a uniform grid spacing of 25 m was selected. For Beberg and for Ceberg the grid spacing was 35 m. For practical reasons it has not been possible to compare with a smaller grid size at any of the sites.

Boundary condition

Boundary conditions are generally obtained from the regional scale models. As there are variants of regional scale models there is also a possibility for selection of which regional variant to use. For all variants Walker and Gylling (1998), Gylling et al. (1999a) and Walker and Gylling (1999) strive to find the regional variant, which most closely resembles the conditions of the site scale model.

For the Aberg base case Walker and Gylling (1998) select boundary conditions, in the form of specified head taken from a special simulation of the model by Svensson (1997a) assuming no density stratification and assuming homogeneous porous medium and fracture zones. The importance of different boundary conditions are explored by analysing a single realisation of the Aberg model with different boundary conditions:

1.1 specified head from a deterministic - homogeneous regional model of Aberg with fresh water conditions (i.e. base case),

1.2 specified head application taken from environmental heads calculated from the reference case of Svensson (1997a) assuming density dependent flow and a heterogeneous medium,

1.3 specified head taken from a realisation of Svensson (1997a) with heterogeneous medium but no salinity,

1.4 directly apply the observed water table and sea level and assume hydrostatic conditions.

The results of these different boundary conditions are that the first three conditions result in relatively similar flow fields, whereas the last condition results in much less flow (order of magnitude lower). Based on these results it appears motivated to accept the base case boundary condition as a *reasonable estimate* and not to further propagate the other boundary condition variants since they all results in equal or much less flow. This also means that the regional flow is important also for site scale hydrogeology. Omitting this coupling would potentially have underestimated the groundwater flow by an order of magnitude. For other site scale model variants (see below) the regional model selection is adjusted to the choice of site scale hydraulic conductivity model as already mentioned.

For the Beberg base case Gylling *et al.* (1999) use the regional scale "Alt K with no density effect" variant (Hartley *et al.*, 1998) as boundary condition. At present there is density stratification at depth, but the base case variant is assumed to better represent future conditions, where the saline water interface will move to greater depths. Present day conditions is represented by *variant 1*, which takes boundary conditions from the density varying Alt K case of Hartley *et al.* (1998) expressed as *environmental head.* Also variant 3 of Gylling et al. (1999a) uses environmental head boundary conditions from Hartley *et al.* (1998), but using their "base case". (The latter has a deviating assumption on the depth dependence of the hydraulic conductivity of fracture zones, see below). For other site scale model variants (see below) the regional model selection is adjusted to the choice of site scale hydraulic conductivity model (with no density stratification) as already mentioned.

For the Ceberg base case the regional specified pressure variant GRST (Boghammar *et al.*, 1997) is used. No other boundary condition variants are explored. This decision finds support from the results of analyses of the Aberg boundary condition variants. For other site scale model variants (see below) the regional model selection is adjusted to the choice of site scale hydraulic conductivity model. For Ceberg variant 1 the fracture zone properties in the regional model was also increased by a factor of 100. For variant 2 the regional model was modified to incorporate the regional additional structures suggested by Saksa and Nummela (1998).

Hydraulic conductivity field

The base case suggestions by Walker *et al.* (1997) are used as base case assumptions for the hydraulic conductivity field. However, for Beberg and Ceberg there is a need to adjust the geostastical model to the 35 m grid scale, since the base case suggested by Walker *et al.* (1997) (see section 6.3) is given for a scale of 25 m. In addition, several variants, suggested either by Walker *et al.* (1997, see section 6.3) or by Saksa and Nummela (1998) are analysed in order to explore uncertainties in hydraulic conductivity.

For Aberg Walker and Gylling (1998) consider an *upscaling* variant where the cell size is increased from 25 m blocks to 50 m blocks and where the median and variance of the hydraulic conductivity are upscaled to this size using the rule suggested by Walker *et al.* (1997). Generally, the variant results in fairly similar flow properties as the base case, an increase of median darcy velocities at deposition hole locations by a factor of 2, but a slight decrease in variance (see also tables 7.2.1 and 7.3.2). While Walker and Gylling (1998) suggest these differences to be unsatisfactory it should instead be emphasised that they are relatively small in relation to the general uncertainty in hydraulic conductivity. Upscaling variants have not been explored for Beberg or Ceberg.

For Aberg Walker and Gylling (1998) explore a variant assuming an *anisotropic covariance of log K*. The choice to change the covariance structure rather than to directly introduce an anisotropic hydraulic conductivity is driven by the limitations in the current version of the HYDRASTAR model. This means that it is not possible to exactly mimic the suggestions by Rhén *et al.* (1997), but the variant would still provide some indication of the significance of hydraulic anisotropy. The resulting flow is in fact quite similar to the base case as can be seen in tables 7.2.1 and 7.3.2. For this reason anisotropic variants have not been analysed for Beberg or Ceberg.

For Aberg Walker and Gylling (1998) also explores two coupled variants assuming *a pure geostatistical model* with a variogram fitted to all measured hydraulic conductivity data, i.e. with no separation between rock domains and conductor domains. A case with no-conditioning and a case with conditioning with respect to measured hydraulic conductivities are analysed. The resulting groundwater flow is around a factor of 5 higher than for the models with different conductor domains (see tables 7.2.1 and 7.3.2). The difference between non-conditional and conditional simulations is relatively minor. Such variants have not been pursued for Beberg and Ceberg, since they must be regarded to be less realistic than the base case.

Conditioning on head is not tried, since the natural head field is very insensitive to the permeability field. The results of such a conditioning would thus be highly questionable. The option is also very resource (i.e. CPU) demanding.

For Beberg variant 2 Gylling *et al.* (1999) explores the consequence of considering the additional fracture zones suggested by Saksa and Nummela (1998). Beberg variant 3 assumes a depth reduction of the fracture zones hydraulic conductivity according to the alternative favoured by Hartley at al. (1998) – i.e. their “base case”. This variant also takes environmental head boundary conditions from the corresponding regional variant.

For Ceberg there is a ”what-if” case (variant 1) with two orders of magnitude increase in conductivity contrast for the fracture zones. Walker and Gylling (1999) note that although the *reasonable estimate* values are based on the on-site hydraulic tests, the low contrast between fracture zones and rock mass is unusual in comparison to other sites. There also are some indications that the zones could be very conductive even if the median conductivity is very low.

Another variant considered at Ceberg (Ceberg variant 2) is to include alternative fracture zones, as suggested by Saksa and Nummela (1998) combined with increased fracture zone hydraulic conductivity. Finally, Walker and Gylling (1999) also consider a “what-if” variant with increased variance of log Hydraulic Conductivity (Ceberg variant 3).

For comparison Walker and Gylling (1998), Gylling et al. (1999a) and Walker and Gylling (1999) also calculate a variant with *deterministic and homogeneous hydraulic conductivities*. The hydraulic conductivity, which has no heterogeneity is derived by applying the upscaling relation suggested by Walker *et al.* (1997). The difference between conductor domains and rock domains is still upheld. For all sites the median flow is quite close to the base case median flow, but the variance is reduced as expected (see table 7.2.1 and table 7.3.2). Allowing for heterogeneous (and uncertain) rock domain hydraulic conductivity results in flow paths with about 5 times higher flux compared to a case with homogeneous (and deterministic) hydraulic conductivity.

Flux consistency

Walker *et al.* (1997) suggest to calibrate the site scale model hydraulic conductivity such that the site scale models reproduce fluxes calculated by the regional models. The approach has the benefit of making the flow consistent in the site and regional scale models. However, as discussed in section 6.3.3, the basic scaling relation used both in the regional scale and site scale are uncertain and it appears quite arbitrary to select the regional scale flow to represent reality since it could just as well be the other way around.

Recognising this Walker and Gylling (1998), Gylling et al. (1999a) and Walker and Gylling (1999) only compare the boundary fluxes in the site and regional scale models respectively. For the base case of Aberg (see section 6.5) they found that the boundary fluxes deviated a factor of 0.5 (with higher fluxes in the regional model). The boundary fluxes in other variants, apart for the homogeneous - deterministic variant, are similar to the base case ones. It is possible that the hydraulic conductivities of the regional model (or the site scale model) could have been adjusted to make the flows even more equal, but also the small deviation found is in fact quite re-assuring considering other potential sources of errors. For Ceberg the orientation of fluxes agree well, but the magnitude of the fluxes deviate much more and the regional model overpredicts the fluxes through the site scale model by a factor of 20. Walker and Gylling (1999) note that this deviation does not fully support the validity of the nested modelling and the associated upscaling, but the boundary flux calculation may suffer from interpolation errors. However, to further investigate the boundary fluxes, Walker and Gylling (1999) also constructs a mass balance for a reduced domain that omits the upper 200 m of the site-scale domain (i.e., the upper surface of the mass balance control volume is lowered to –100 masl for both models). The net inflow and outflow over the site-scale domain for the regional and site-scale models are within 40%, suggesting that most of the discrepancy between the nested models occurs near the upper surface of the domain. The flow in these regions are not of primary interest to the safety assessment.

6.5.4 Alternative models for the detailed scale hydrogeology

SR 97 also includes an “Alternative Model Project” (Selroos and Ström, 1999) for exploring the uncertainty implied by the conceptual uncertainty in the description of the conductive medium. The AMP project applies a stochastic continuum (Widén and Walker, 1999), a discrete fracture network (Dershowitz *et al.*, 1999) and “channel network” (Gylling *et al.*, 1999b) on a subsection of the Aberg local model region. All three models apply the same boundary conditions, derived from the non-density case of Svensson (1997a). The input data needs for the CHAN3D model is essentially the same as for the HYDRASTAR model, as already discussed in section 6.3. The discrete fracture network model requires fracture size, orientation, intensity and transmissivity data (for details, see Dershowitz *et al.*, 1999).

Another alternative model is presented by Svensson (1997b). He essentially uses the Aberg base case hydrogeological parameters, but also considers the effect of salinity on the site scale flow. This essentially results in a one order of magnitude reduction of the darcy velocities at the repository level (see table 7.2.2). It could, however, be argued that the assumption of a stationary salinity field is unrealistic given the progressive land-rise (Voss and Andersson, 1993) and that higher flows may result if the moving boundary was considered. Consequently, it cannot directly be stated that the model by Svensson (1997b) is more realistic that the base case model of Walker and Gylling (1998).

The SKI performance assessment exercise SITE-94 (SKI, 1996) involved extensive flow modelling of Äspö. This modelling involved both a discrete network and a stochastic continuum approach. Several variants, formulated to handle concerns and uncertainties were explored.

It should be noted that these alternative modelling exercises of the Aberg site are not fully comparable and are not fully comparable to the stochastic continuum modelling presented by Walker and Gylling (1998). The input information, boundaries and modelling objectives considered differ. For consistency, the SR 97 flow related migration parameters, which are discussed and selected in chapter 7, are primarily to be derived from the Walker and Gylling (1998), Gylling et al. (1999a) and Walker and Gylling (1999). The results of the alternative models are, however, considered when discussing the realism and conservatism of parameter selection.

6.5.5 Quantification of uncertainties

Table 6.5.1 summarises the analysed quantification of uncertainties in the site scale hydrogeological models.

Table 6.5.1 *Analysed quantification of uncertainties in site scale hydrogeological models*

Case	Aberg	Beberg	Ceberg
Reasonable estimate	Aberg base case as defined by Walker and Gylling (1998).	Beberg base case as defined by Gylling *et al.* (1999a).	Ceberg base case as defined by Walker and Gylling (1999).
Variants	1. Boundary conditions 2. Upscaling of LogK 3. Anisotropic Covariance of log K 4. Conditional Simulation of log K 5. Deterministic Simulation DFN-model (Dershowitz *et al*, 1999), Channel Network model (Gylling *et al.*, 1999b), Saline model (Svensson 1997b). The latter for qualitative assessment.	1. Environmental head B.C. 2. Additional fracture zones 3. Alternative interpretation of depth dependence and environmental head B.C. 4. Deterministic	1. Increased Fracture Zone contrast 2. Alternative fracture zones 3. Increased variance 4. Deterministic Simulation

7 Flow related migration parameters

Several important parameters needed for the *near-field* release and *far-field* migration calculations directly depend on different aspects of the groundwater flow field. For simplicity these parameters are called flow related migration parameters. However, before discussing how to obtain parameters to these models it is necessary to derive an approach to *handling spatial variability* in the results of the groundwater flow modelling.

7.1 Handling spatial variability

7.1.1 Introduction

As already discussed in chapter 6, the groundwater flow in crystalline media varies considerably in space. There are at least three issues that need to be handled in relation to selection of migration parameters from a spatially varying flow field. These are:

- handling of multiple realisations,
- selection of *reasonable estimate* and pessimistic values in a spatially varying field,
- the emplacement strategy.

No specific study on emplacement strategy is conducted within the framework of SR 97. Rather, the results of SR 97 may be used as input information when developing such a study. The SR 97 approach to these issues is addressed in the following.

7.1.2 Handling of multiple realisations

For a single set-up of input parameters the stochastic hydrogeological models result in many different realisations. It should be recognised that the differences within a realisation is an estimate of the spatial variability - not uncertainty - and that this spatial variability would not necessarily be reduced if there was more information. In contrast, differences between different realisations, as well as differences between different variants represent the uncertainty in the knowledge of the site. However, as long as there is only one canister failure at an unknown position, the distinction between uncertainty and spatial variability is inconsequential, the full uncertainty in hydraulic properties of the failed position is obtained from the ensemble statistics. Furthermore, inspecting the predicted differences between different realisations, as depicted in figure 7.1.1, clearly indicates that differences between realisations is small compared to differences within realisations.

Based on the fact that only few canisters will fail and that the position of the failed canister(s) will be unknown it is recommended to base the input to consequence analysis on the *ensemble statistics* of the HYDRASTAR results. Furthermore, it should be noted that this ensemble statistics to a very large extent is *a measure of the spatial variability* of the site even if there also is uncertainty represented by difference in different realisations. The uncertainty in (the stochastic) hydrogeologic properties are described in the difference between different variants.

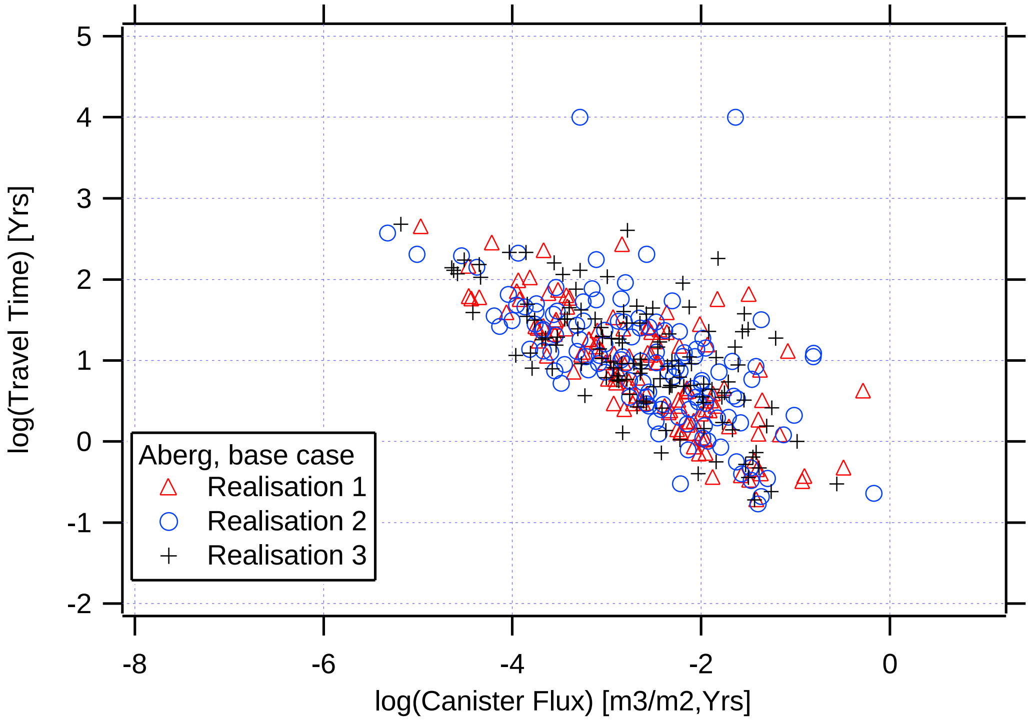


Figure 7.1.1. *Examples of HYDRASTAR realisations for Aberg base case parameters (from Walker and Gylling, 1998).*

7.1.3 Selection of single values in a spatially varying field

The hydrogeologic modelling provides uncertain, spatially varying results. If few canisters fail (at random), the position of these failed canister is completely random and it is not possible to designate the *reasonable estimate* failure positions. As can be seen from figure 7.1.1 the spread of canister fluxes and travel times for a random canister position are quite large and it is difficult to designate a value, which is very much more likely than other values within the range. However, for illustration purposes it is suggested to use median values to represent a "*reasonable estimate*", but is not suggested that they are more likely than other values. An uncertainty analysis needs to consider the full range of the predicted distribution.

With regard to selection of single pessimistic values the procedure is possibly more straightforward. One should find "bad" positions (i.e. high flow and little far-field retention) and also consider different variants. Clearly, this strategy would on one hand not guarantee that the most adverse parameters are found and on the other hand possibly pick out a very unlikely situation. Again, the ”pessimistic” values should rather be seen as illustrations of the consequences of quite pessimistic assumptions.

7.1.4 Canister emplacement strategy

The position of the failed canister(s) is used to find flow related transport parameters from the hydrogeologic analyses to use as input to the migration codes COMP23 and FARF31. Due to the strong spatial variation of the geosphere properties, the consequence of a canister failure may be strongly dependent on the location of the failed canister.

When constructing the repository and when selecting canister deposition holes it is evidently possible to avoid locations which appear to be less favourable. Such active emplacement strategy may thus diminish the significance of the more extreme geosphere properties. However, the impact of the emplacement strategy depends upon the possibilities to actually attribute specific geosphere properties to specific locations, i.e. it depends upon the exploration technique to be used during repository construction. Evaluation of such techniques lies outside the scope of SR 97. Instead the approach suggested is to explore the potential significance of such techniques.

Suggested quantification

When discussing an active emplacement technique it is necessary to assess which geosphere properties that can be measured and thereby avoided. Already the means of deriving repository layout where major fracture zones are avoided (see section 6.2) implies important credit to active emplacement. In addition, it does not seem unrealistic that it will be possible to fairly accurately determine the hydraulic properties around deposition holes.

The attainable precision in determination of deposition hole characteristics is still subject to investigation (e.g. Dahlström, 1998). However, in order to study the potential significance of avoiding ”bad holes” one may formulate emplacement criteria in terms of the maximum acceptable darcy velocity in the deposition hole scale. This darcy velocity is readily obtained from the detailed scale.

At present there seems to be little possibility to identify the migration paths for a specific deposition hole or biosphere release point. However, only migration paths starting in deposition holes with accepted deposition hole scale darcy velocity should be analysed. This means that the deposition hole selection criteria may affect the selection of far-field migration paths and biosphere release points in cases where there is correlation between near-field fluxes and far-field migration properties.

Given the lack of information it seems most appropriate to consider the case *without credit* for active emplacement (apart from the already given repository layout) as both the *reasonable estimate* and *pessimistic* cases of emplacement technique.

The potential significance of active emplacement could be explored as variant cases. The general technique would be to exclude deposition holes (and connected migration paths if applicable) if darcy velocity in this scale exceeds a certain value. At a first instance such considerations should be made on the performance measures calculated from the detailed scale hydrogeologic models (i.e. q_{nf}, F, biosphere release points), see section 7.3. The effect on q_{nf} is of course obvious, but the effect on F and biosphere release point will depend on the correlation between q_{nf} and the other parameters.

7.1.5 Summary of suggested strategy

Table 7.1.1 summarises the above suggestions.

Table 7.1.1: *Suggested handling of spatial variability*

Case	Description
Reasonable estimate	Use ensemble statistics to cover spatial variability and related uncertainty. Select median for single value illustration. Do not take credit for emplacement strategy
Pessimistic	Combine the pessimistic near-field, far-field and biosphere parameter values (i.e. assume full correlation between all unfavourable conditions). Do not take credit for emplacement strategy.
Variants	Consider different variants, but still use ensemble statistics to cover spatial variability. As a "what-if" case explore effect of excluding deposition holes (and connected migration paths if applicable) if darcy velocity in this scale exceeds 10^{-1} m/yr, 10^{-2} m/yr or 10^{-3} m/yr.

7.2 Near-Field - COMP23

7.2.1 Source of information

The results of the repository scale stochastic continuum groundwater flow simulations presented by Walker and Gylling (1998), Gylling et al. (1999a) and Walker and Gylling (1999) constitute the prime source of information to the flow related near-field migration parameters. Additional flow information is given within the framework of the AMP-project (Widén and Walker, 1999, Dershowitz *et al.*, 1999, and Gylling *et al.*, 1999b) as well as by separate flow calculations performed by Svensson (1997b).

Moreno and Gylling (1998) complemented by Andersson *et al.* (1998) discuss how to obtain near-field rock migration path parameters to the near-field release model COMP23 (Romero, 1995) using results from the detailed scale hydrogeological analyses. Andersson *et al.* (1998) also suggest values of flow porosity based on an evaluation of tracer tests results from the different sites. Rhén (1998) provides information on the excavation damaged zone (EDZ) based on the ZEDEX experiment (Olsson *et al.,* 1996) conducted at Äspö (i.e. Aberg). Pettersson et al., (1999) explores the potential impact of flow in the backfill. Finally, Lindgren and Widén (1998) explore the degree of discretization needed in the model.

7.2.2 Use in SR 97, modelling approach and conceptual model uncertainties

The near-field code COMP23 builds on the NUCTRAN code (Romero, 1995). NUCTRAN calculates the non-stationary nuclide transport in the near field of a repository. The system is divided into compartments, where the only restriction is that a compartment is formed of the same material. The model, which is a very coarsely discretised Integrated Finite Difference Model, embeds analytical solutions at locations where other models require a very fine discretisation such as entrances and exits from small holes and fractures. In the repository, radionuclides leaking out through a small hole in the canister wall diffuse into the clay and may then migrate through various pathways into the flowing water in rock fractures.

In its present conceptualisation COMP23 (Romero, 1995) considers release through four different pathways from the canister deposition hole and out to the ”far-field rock”. These are:

- Q1: direct release into a fracture intersecting the canister deposition hole ,
- Q2: release into a disturbed zone thought to exist at the floor of the deposition tunnel,
- Q3: release into a fracture zone intersecting the tunnel backfill,
- Q4: diffusion through the rock mass followed by release into a fracture zone close the deposition hole, but not intersecting it.

These pathways are schematically illustrated in figure 7.2.1.

For each such potential pathway Moreno and Gylling (1998) show how to derive an ”equivalent flow”, $Q_{eq,i}$ which describes the mass transfer from the COMP23 compartment into the far-field. According to Moreno and Gylling (1998),

$$Q_{eq,i} = 2W_i\sqrt{4D_w q_i L_i \varepsilon_i / \pi} \qquad (7.2.1)$$

where W_i is the width of the fracture surface in contact with the flowing water, D_w the diffusivity in water, q_i is the darcy velocity, L_i the length of the pathway in contact with water and ε_i the flow porosity of the respective pathways. The properties which determine $Q_{eq,i}$ are generally different for each pathway, but presently when assessing HYDRASTAR flow solution only the darcy velocity in scale of the calculation model blocks (q_0) is obtained from this flow solution, whereas the darcy velocities to be used by COMP23 are derived as different multiples of q_0. Under this assumption Moreno and Gylling (1998) also introduces the parameter f_i and A_0 where

$$Q_{eq,i} = f_i \sqrt{q_0} A_0$$

and A_0 is defined for a situation where the flow porosity of the rock surrounding the deposition hole is 0.0001, the width of the contact surface area is 5 m (the canister height) and the path length is 2.75 m. (The parameter f_i is used for convenience in COMP23, but the important parameters for determining Q_{eq} are q_i, ε_i, L_i and W_i).

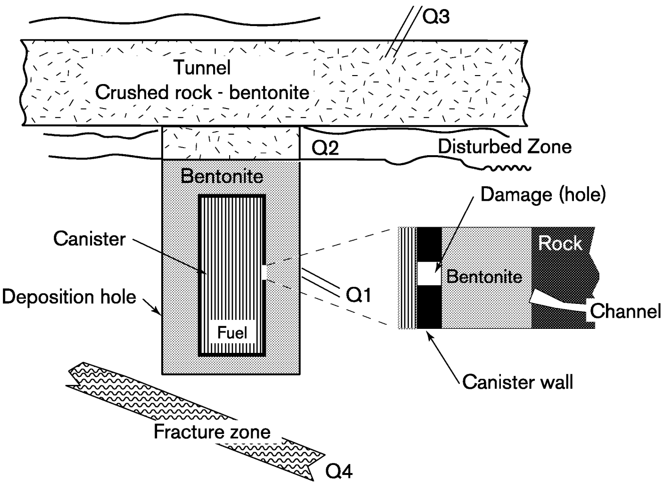


Figure 7.2.1: *Schematic illustration of the different release pathways considered by COMP23 (from Moreno and Gylling, 1998).*

The detailed groundwater flow analyses using the discrete network or channel network approaches can in principle provide consistent estimates of the pathways in the near-field scale and how these are connected to the far-field. For example, the field data now collected within the framework of the Äspö TRUE Blockscale experiment (Winberg, 1997) could be used to study this. In particular since the evaluation of experimental data is used to construct a discrete fracture network of the site. Such information cannot be used fully in the present conceptualisation of COMP23. Exploration of the possibilities of providing more realistic input to the COMP23 pathways from the detailed scale hydrogeological models could be contemplated as a research option, beyond SR 97. A proper coupling between the near-field and far-field migration, using the predicted flow paths from hydrogeology could be contemplated. For SR 97 the approach has to be to select values for the darcy velocities in the different pathways that both can find support from data and also would err on the pessimistic side, i.e. if anything overestimate the release into the far-field.

Another, related problem, not fully properly handled presently, is the fate of releases through the Q2-Q4 pathways. In principle they may experience far-field migration properties that deviate from those released directly through the Q1 pathway. However, the Q3 and Q4 pathways are generally quite insignificant and given the relatively coarse resolution of the flow field obtained from the HYDRASTAR solution there is in practice no possibility to separate between the far-field component of the Q1 and Q2 pathways. This implies that the concern is of second order, but could be more significant in case a more detailed resolution of the near-field flow and transport were to be modelled in future assessments.

An important assumption in the present conceptualisation of COMP23 is that diffusion and not advection drive migration in the backfill. However, it is not certain that there will be no groundwater flow in the backfill (see also section 5.4). In order to address this problem Pettersson *et al.* (1999) explore the potential effects of flow in the backfill by a special model exercise. They conclude that the impact of flow has little influence on the release since the main transport resistance in the near-field is not located in the tunnel. If the canister damage is small, the release will be controlled by the release through the hole; for larger canister damage the bentonite buffer will control the release. At most the release increases a factor of two for a few nuclides.

Lindgren and Widén (1998) explore the degree of discretisation needed in the model. By following their recommendations, the discretisation errors can be neglected in relation to other uncertainties.

7.2.3 Data uncertainties, correlation and dependencies on other parameters

With the current conceptualisation the following data uncertainties and correlation to other parameters should be considered for the near-field migration paths:

- uncertainty and spatial variability in darcy velocity,
- uncertainty in Darcy velocities in different COMP23 pathways,
- uncertainty in porosity,
- geometry of interface between near-field and far-field,
- the potential correlation between near field flow and retention properties of the far-field migration paths.

Uncertainty and spatial variability in darcy velocity

The uncertainty and spatial variation in groundwater flow at the scale of the resolution of the stochastic continuum representation (i.e. q_0) is handled by the different model variants and multiple realisations of the stochastic detailed scale hydrogeology discussed in section 6.5. Table 7.2.1 displays the results of the calculations made by Walker and Gylling (1998), Gylling et al. (1999a) and Walker and Gylling (1999). Furthermore, as already discussed in section 7.1 the ensemble statistics is a good representation of the spatial variability of the flow field, which means that only ensemble values are presented here. The following may be observed from table 7.2.1.

- For Aberg most variants are very similar to the base case. The variants without structures are not really physically motivated and could thus be discarded (their deviation from the base case is also relatively minor). However, the anisotropy variant shows a slightly higher maximum darcy velocity. This needs to be considered as a pessimistic value.

- Also for Beberg most variants are similar to the base case, which thus could be the basis of a *reasonable estimate*. However, the flow (also the percentiles) is about a factor of two lower in the variant (variant 3) assuming a more pronounced depth decrease combined with density stratification. There is also slightly higher flow in the homogeneous - deterministic variant.

- For Ceberg most variants are similar to the base case. The variant with additional conductor domains and increased hydraulic conductivity in the conductor domain shows a factor of ten higher maximum darcy velocity. This variant is however, quite extreme as it is based on a "what-if" suggestion. The only pessimistic value, which could find support in the data, would be to take the 95% of the base case value.

It could also be noted that the darcy velocity of Aberg and Beberg is almost two orders of magnitude higher than the darcy velocities of Ceberg. Most of this difference can probably be directly related to the suggested difference in hydraulic conductivity of the sites (see Walker *et al.*, 1997 and table 6.3.1).

Table 7.2.1 *Distribution of log scale (base 10) darcy velocities (m/yr) in deposition hole scale obtained from detailed scale hydrogeologic analyses by Walker and Gylling, (1998), Gylling et al. (1999a) and Walker and Gylling (1999).*

Case	***Median***	***5%***	***95%***
Aberg			
Base case	-2.7	-4.5	-1.3
Environmental head B.C[1].	-2.7	-4.5	-1.3
Upscaling	-2.4	-3.8	-1.3
Anisotropy	-2.7	-4.6	-1.1
No structures	-2.2	-3.9	-0.8
No structures and conditioning	-2.1	-3.8	-0.6
Deterministic – Homogeneous	-2.7	-3.4	-2.1
Beberg			
Base case	-2.9	-3.9	-1.8
Environmental head	-2.7	-3.7	-1.7
Additional zones	-3.0	-3.9	-1.8
Alt. depth dependence + envin. BC	-3.2	-4.2	-2.1
Deterministic – Homogeneous	-2.7	-3.0	-2.3
Ceberg			
Base case	-4.5	-5.2	-3.8
Increase K in CD	-4.4	-5.1	-3.7
Additional CD and increased K in CD	-4.4	-5.1	-2.7
Increased variance in both RD and CD	-4.3	-5.3	-3.5
Deterministic – Homogeneous	-4.5	-4.6	-4.3

[1] Based on a single realisation.

It is also worthwhile to consider whether other model approaches would result in different results. As already discussed in section 6.5.4 there exist several different modelling exercises of Aberg. Table 7.2.2 displays the darcy velocity distributions resulting from these different analyses. It should be understood that the results of table 7.2.2 are not fully comparable, but tentatively the following conclusions may be drawn:

- both median and ranges are fairly similar in most analyses,
- the high flow (95%) of the flowing positions of the discrete network analysis (DFN) is a factor of 10 higher than the high flow of the stochastic continuum analyses,
- the discrete network analysis (DFN) also results in a large number of holes (59%) with no flow at all.

Table 7.2.2 *Distribution of log darcy velocities (m/year, log scale) in deposition hole scale at Aberg for the base case in other analyses. (The different analyses are not fully comparable)*

Case	***Median***	***5%***	***95%***
Base case (Walker and Gylling, 1998)	-2.7	-4.5	-1.3
HYDRASTAR, AMP (Widén and Walker, 1999)	-3.2	-5.0	-1.5
DFN (Dershowitz *et al.,* 1999)[1]	-3.2	-5.2	-1.9
CHAN3D, (Gylling *et al.* 1999b)	-3.3	-4.0	-1.7
SKI SITE-94[3], (SKI, 1996)	-2.8	-5.0	-1.0

[1] On average 59% of deposition holes in the DFN analysis had no flow at all. These holes are excluded from the above statistics.[2] Results are approximate for "sector 6", table 5-21 in Dershowitz *et al.* (1999). [3] Various approaches.

In general these observations indicate that the present stochastic continuum evaluation of the sites provided a fair representation of the groundwater flow at the sites. Furthermore, the difference between the stochastic continuum results, representing a scale of 25 m - 35 m blocks, and the Discrete Network results, which are evaluated on the scale of individual deposition holes, could be used as an indication on how to transfer the stochastic continuum model scale darcy velocities to darcy velocities of the deposition hole scale.

In summary the following suggestions seems highly motivated:

- select the base cases of Aberg, Beberg and Ceberg respectively as the *reasonable estimates* of the flow and the median of these base cases as the *reasonable case single value* (Aberg $q_0=2\cdot10^{-3}$ m/yr, Beberg $q_0=1\cdot10^{-3}$ m/yr and Ceberg $q_0=4\cdot10^{-5}$ m/yr) illustrations for these sites,
- select the (95%) maximum darcy velocities of the anisotropy variant for Aberg ($q_0=10^{-1}$ m/yr), the environmental head variant for Beberg ($q_0=2\cdot10^{-2}$ m/yr) for Beberg and the base case for Ceberg ($q_0=2\cdot10^{-4}$ m/yr), as pessimistic values of the darcy velocities,

- consider the full range spatial variability of the respective base cases for probabilistic analyses (since the most variants are quite similar to the base case).

Darcy velocities in different COMP23 pathways

The detailed scale hydrogeology analyses provide groundwater flow over a certain average area. The darcy velocities calculated by Walker and Gylling (1998), Gylling et al. (1999a) and Walker and Gylling (1999) represent an average over the cell size (25 m to 35 m grid spacing) and there is no further information of the variability of the scale of the deposition hole (or for individual fractures intersecting the hole) or for the other pathways handled in COMP23.

For the Q1 pathway (directly from deposition hole to a fracture in the rock) the averaging will result in some reduction of the spatial variability of the flow. Comparison between near-field darcy velocities estimated by Widén and Walker (1999) and estimated from the discrete fracture network analysis of Dershowitz *et al.* (1999) (see table 7.2.2), suggests that the median flows are rather similar. It is suggested to use $q_1=q_0$ as a *reasonable estimate*, but to assume $q_1=5q_0$ as a pessimistic value. Lacking analyses of Beberg and Ceberg it is suggested to apply this suggestion to these sites as well. Furthermore, the discrete network approach provides estimates of the number of deposition holes not directly intersected by flowing fractures (i.e. where $q_1=0$). Even if only 41% of the positions flow in these analyses the probability is still large to hit a flowing hole. Nevertheless, it may be worthwhile to consider a case with $q_1=0$, but q_2-q_4 flowing as a variant to study significance of ”dry” holes.

The hydraulic implication of the excavation-damaged zone, if it exists, has already been discussed in section 6.5. Both Walker *et al.* (1997) and Rhén (1998) suggest that there is fairly little quantitative information regarding the hydraulic properties of the excavation-damaged zone (EDZ). It is, however, possible to draw some conclusions from the ZEDEX experiment (Olsson *et al.*, 1996, vol 1) carried out at Äspö. It can be concluded that:

- it is not clear that the EDZ will imply permeability changes,
- only minor hydraulic impacts can be expected in full face bored tunnels (TBM),
- for a conventional tunnel, with drill and blasting technique (DB), a variation case with a 100 times increase in hydraulic conductivity in a 1 m deep zone below the tunnel bottom could possibly be motivated.

Even if the EDZ exists it does not affect the overall flow, but it may redistribute the flow in the tunnel scale making the darcy velocity in the EDZ (q_2) larger than the darcy velocity directly around the deposition hole (q_1). As a *reasonable estimate* for a DB tunnel it is suggested to assume $q_2=10q_0$. However, at the extreme, this redistribution is in the same order as the hydraulic conductivity increase, but will in reality always be lower. A clear overestimation of the effect of a 100 times permeability increase in the EDZ would be to assume $q_2=100q_0$.

Through sensitivity calculations Romero *et al.* (1996) show that the Q_1 and Q_2 pathways dominate (if they exist) for almost any choice of q_3 and q_4, the reason being that the migration resistance is controlled by the canister and the buffer. This means that the proper selection of darcy velocities for Q_3 and Q_4 is not very important and pessimistic high values could be selected without biasing the function of the near-field. However, it would indeed be desirable to include realistic estimates of these flows in order not to confuse the hydrological description of the site, but also in case alternative scenarios may change the relative importance of these pathways. It is suggested to use $100q_0$ as *reasonable estimate* for both q_3 and q_4 and to use $q_3=1000q_0$ and $q_4=10000q_0$ as very pessimistic estimates.

Porosity

Andersson *et al.* (1998) note that tracer tests conducted at Aberg and Beberg suggest that a median value of the flow porosity, both at Aberg and Beberg is 10^{-3}. The range is large and is a result both of spatial variability and pure uncertainty. The high porosity seems improbable for a selected deposition hole and thus 10^{-4} is selected as a *reasonable estimate*, but the higher value 10^{-3} should be selected as a pessimistic value. Lacking other information it is suggested to use these values at Ceberg as well.

There are no real data on the EDZ porosity. It seems justified to assume them to be higher than the deposition hole rock porosity. For a *reasonable estimate* $\varepsilon_2= 3\cdot10^{-4}$ is suggested, but a pessimistic value would still be $\varepsilon_2=10^{-3}$.

Andersson *et al.* (1998) conclude that currently there is no clear experimental support for assigning different values of flow porosity (ε_f) to different parts of the rock (such as major fracture zones and the rock between these fracture zones), but there are indications that porosity generally increase with permeability. For this reason it is suggested that porosity in the Q3 and Q4 paths are one order of magnitude higher than in the other paths, i.e. $\varepsilon_3=\varepsilon_4=10^{-3}$ for all cases and sites.

Diffusivity

Ohlsson and Neretnieks (1997) report values of diffusion in water for radionuclides in the range from $0.15\text{-}2.0\cdot10^{-9}$ m^2/s. For radionuclides where data is lacking it is assumed that $D_w = 1\cdot10^{-9}$ m^2/s. Due to the many uncertainties in other data Moreno and Gylling suggest using $D_w = 1\cdot10^{-9}$ m^2/s for all radionuclides within SR 97.

Geometry of interface between near-field and far-field

Table 7.2.3 lists values of W_i and L_i suggested by Moreno and Gylling (1998). Lacking a detailed evaluation of the near-field/far-field interface it is suggested to use the values in SR 97.

Table 7.2.3 *Values of W_i and L_i to be used in COMP23 (for definitions see Moreno and Gylling, 1998).*

Path	W_i (m)	L_i (m)
Q1	5	2.8
Q2	1	2.8
Q3	2.5	7.0
Q4	2.5	5.0

Correlation between near-field and far-field

Another issue worth commenting on is the potential correlation between near field flow and retention properties of the far-field migration paths. It seems reasonable that high q_{nf} should be correlated to low F values and such a correlation can also be seen in the results of the analyses by Walker and Gylling (1998), Gylling et al. (1999a) and Walker and Gylling (1999) (see e.g. figure 7.1.1). Exploring such a correlation would potentially be important for the total consequences but is also important for assessing the potential gains of an active canister emplacement policy. For HYDRASTAR results this is not a modelling problem as long as near-field flow and far-field migration parameters are taken from the same realisation and the same deposition hole. Then this correlation is taken care of automatically.

Another, but connected problem, is the derivation of the far-field migration properties connected to the Q2-Q4 paths. They may deviate substantially from those of the direct path, but the spatial resolution of the stochastic continuum model does not make more detailed analyses possible. However, these paths are only significant if the Q1 path is of second order.

7.2.4 Summary of quantification of uncertainties

Table 7.2.4a summarises the above suggestions regarding the near-field darcy velocities at the different sites. Table 7.2.4b summarises the suggestions for the non-site specific parameters.

Table 7.2.4a *Quantification of uncertainties in near-field flow Darcy velocity q_0 (m/yr)*

Case	Aberg	Beberg	Ceberg
Reasonable estimate	$2 \cdot 10^{-3}$	$1 \cdot 10^{-3}$	$4 \cdot 10^{-5}$
Pessimistic	10^{-1}	$2 \cdot 10^{-2}$	$2 \cdot 10^{-4}$
Probabilistic	Explore range of Aberg base case (Walker and Gylling, 1998)	Explore range of Beberg base case (Gylling et al., 1999a)	Explore range of Ceberg base case (Walker and Gylling, 1999)

Table 7.2.4b: *Non site specific parameters for input to COMP23*

Parameter	***Reasonable estimate***	***Pessimistic***
Darcy velocities		
q_1	q_0	$5q_0$
q_2	$10q_0$	$100q_0$
q_3	$100q_0$	$1000q_0$
q_4	$100q_0$	$10000q_0$
Porosity		
ε_1	10^{-4}	10^{-3}
ε_2	$3 \cdot 10^{-4}$	10^{-3}
ε_3	10^{-3}	10^{-3}
ε_4	10^{-3}	10^{-3}
The "f_i" parameter in COMP23		
f_1	1	7
f_2	2	13
f_3	25	80
f_4	21	220

7.3 Far- field - FARF31

7.3.1 Source of information

The results of the repository scale stochastic continuum groundwater flow simulations presented by Walker and Gylling (1998), Gylling et al. (1999a) and Walker and Gylling (1999) are also the main source of information for the flow related far-field migration parameters. Additional flow information is given within the framework of the AMP-project (Widén and Walker, 1999, Dershowitz *et al.*, 1999 and Gylling *et al.*, 1999b) as well as by separate flow calculations performed by Svensson (1997b). In addition Andersson *et al.* (1998) suggest estimates of the flow wetted surface and some related parameters. The site-specific information builds on some tracer tests, geological characterisation, hydraulic measurements, and modelling, but several assumptions are needed in order to handle the lack of adequate data for some of the parameters.

7.3.2 Use in SR 97, modelling approach and conceptual model uncertainties

Radionuclide migration through the geosphere is primarily modelled with the one-dimensional code FARF31 (Norman and Kjellbert, 1990). A FARF31 solution is adjusted to each flow tube produced in order to represent the spatially varying flow field. FARF31 considers advection and dispersion along the migration path, matrix diffusion and sorption transverse the path and chain decay.

The direct input parameters to FARF31 are the total migration time t_{tot}, the flow wetted surface per volume of water $a_{w,glob}$ and the ”Peclet”-number. The Peclet number is given by,

$$Pe = L \cdot v/D$$

where L is the migration length, v is the advective velocity and D is dispersivity. However, it needs to be stressed that the “travel time” alone has very little impact on the resulting retention. Andersson *et al.* (1998) demonstrate that the assessment relevant parameter for migration modelling of sorbing elements is the ”F-quotient”,

$$F=a_r \cdot L/q$$

where a_r is the flow wetted surface per volume of rock, L is the migration path length and q the Darcy velocity. However, F could also be expressed as

$$F=a_w \cdot t_w$$

where t_w is the “transit time” and a_w is the “flow wetted surface per volume of water”. The ”F-quotient” for a migration path made up of many small segments each with different flow and geometry is simply the sum of the F-quotients for the individual segments, or more generally the integral along a migration path with varying parameters (Selroos and Cvetkovic, 1996).

There are several conceptual model uncertainties associated to the present modelling of radionuclide migration including:

- the fact that flow is not evenly distributed between different fractures and migration paths makes the concept of a ”global” flow wetted surface improper,
- the effect of diffusion into stagnant or low flow zones in a single fracture,
- other errors involved in abstracting three-dimensional flow information into a set of one-dimensional flow tubes.

In addition to the direct recommendations for SR 97 Andersson *et al.* (1998) also strongly recommended that special analyses are initiated, which may resolve some of the above issues and thus allow more precise estimates of migration parameters in future analyses.

7.3.3 Data uncertainties, correlation and dependencies on other parameters

Andersson *et al.* (1998) point out that despite the fact that FARF31 strongly depends on ”*transit time*”(t_w) and ”*flow wetted surface per volume of rock*” (a_w) it is incorrect to conclude that any of these parameters individually are very important. The reason is that a_w, through porosity, is *strongly correlated* to the transit time. The important factor is the product F and this is almost insensitive to porosity since porosity cancels out in the multiplication. Ideally, one would like to estimate the integral of F along migration paths, but since this is not practically possible, Andersson *et al.* (1998) recommend estimating a_r and q rather than a_w and transit time since the former pair depend less on each other.

In theory tracer tests would be very important for determining retention characteristics along migration paths. As discussed by Elert (1997), the reported tracer tests from Aberg and Beberg are, however, not very sensitive to the effect of diffusion into the rock matrix. There are no tracer tests from Ceberg. This means that the retention characteristics need to be obtained indirectly from different sources. With the current conceptualisation the following data uncertainties and correlation to other parameters should be considered:

- uncertainty and spatial variability in flow wetted surface per volume of rock and its correlation to the flow,
- uncertainty and spatial variability in flow porosity,
- uncertainty and spatial variability in groundwater flow for different migration paths,
- uncertainty and spatial correlation in Peclet numbers,
- the potential correlation between flow related migration parameters and properties of the rock matrix.

”Flow wetted surface” per volume of rock along migration paths

Andersson *et al.* (1998) estimate the flow wetted surface per volume of rock a_r (or rather the migration path width per unit rock cross section area) from estimates of the conductive fracture frequency (CFF). The CFF, in turn, is estimated from the number of conductive bore hole test sections in relation to the total number of bore hole test sections. If flow was evenly distributed among all fractures there is a one-to-one relation between a_r and CFF, but in reality only few migration paths carry the majority of flow which means that the CFF overestimates the a_r corresponding to the actual migration paths. This is also indicated by the discrete network analyses conducted by Geier (1996). However, estimating CFF from the number of flowing test sections generally underestimates CFF since it is then assumed that only one fracture per flow test section is responsible for the flow. Andersson *et al.* (1998), thus suggest that the approximation is a fair ”*reasonable estimate*” but suggest a ten times lower value for a pessimistic case.

Applying this technique yields a value of a_r in the order of 1 m^{-1} for Aberg and Beberg, a value of 0.1 m^{-1} for Ceberg. With an uncertainty range of a factor of 10, in both directions Andersson *et al.* (1998) note that these values are not in conflict with the very uncertain estimates from tracer tests or geochemical information from the sites. However, the low a_r value for Ceberg is probably an artefact of the long test section length used there. On the other hand the number of non-conductive 25 m sections are high at Ceberg in comparison to the other sites, and in addition there are no other estimates. Still, it seems unreasonable to further reduce the a_r value for Ceberg, since already the *reasonable estimate* value is quite pessimistic. Table 7.3.1 summaries the above recommendations. Andersson *et al.* (1998) note that there is room for development of more sophisticated techniques of estimating this important migration parameter.

Flow porosity

Andersson *et al.* (1998) note that tracer tests conducted at Aberg and Ceberg suggest that a median value of flow porosity, both at Aberg and Beberg is 10^{-3}. The range is large and is also a result of spatial variability and not pure uncertainty. However, given the fact that the value chosen for the flow porosity does not affect the calculated migration of sorbing radionuclides, provided a_r is kept at desired values, Andersson *et al.* (1998) suggest to only use 10^{-3} in the geopshere migration calculations. Lacking other information they also suggest using these values at Ceberg as well. However, Walker and Gylling (1998), Gylling et al. (1999a) and Walker and Gylling (1999) use a porosity value of 10^{-4} in the HYDRASTAR simulations. Given the relative unimportance of porosity also this report recommends using 10^{-4}, rather than 10^{-3}, since the results of Walker and Gylling (1998), Gylling et al. (1999a) and Walker and Gylling (1999) then could be used without re-scaling. This inconsistency will not affect the release of sorbing radionuclides, but will overestimate the release of non-sorbing ones. Furthermore, it makes the "transit times" presented at least a factor of 10 too short, which should be kept in mind if comparing the results of Walker and Gylling (1998), Gylling et al. (1999a) and Walker and Gylling (1999) with estimates of groundwater ages at the sites.

There is currently no clear experimental support for assigning different values of flow porosity (ε_f) to different parts of the rock (such as major fracture zones and the rock between these fracture zones), but there are indications (Rhén *et al*, 1997). More precise parameter estimates would be needed to further substantiate such a conclusion before it could be considered in performance assessment. It also strongly needs to be pointed out that "migration times" estimated from a velocity field with varying porosity *cannot be used* as input to FARF31. If varying porosities should be used it is necessary to evaluate the integral $F = \int a_r(s)/q(s)ds$ along the migration paths and then apply an $a_w = F/t_w$ in FARF31(see Andersson *et al.*, 1998).

Table 7.3.1: *Suggested values of a_r and flow porosity for use in SR 97 with reasonable estimate and range.*

Type of data	Aberg	Beberg	Ceberg
Flow wetted surface - a_r (m^{-1})			
All domains	1.0 , 0.1	1.0 , 0.1	0.1. 0.1
Values recommended by Andersson *et al.* (1998)	1.0 (10 - 0.1)	1.0 (10 – 01)	0.1 (1. – 0.01)
Flow porosity ε_f			
All domains	10^{-4}	10^{-4}	10^{-4}
Values recommended by Andersson *et al.* (1998)	10^{-3} (10^{-4} - 10^{-2})	10^{-3} (10^{-4} – 10^{-2})	10^{-3} (10^{-4} - 10^{-2})

Groundwater flow, ”transit time” and the F-quotient

The uncertainty and spatial variation in groundwater flow for different migration paths is handled by the different model variants and multiple realisations of the stochastic detailed scale hydrogeology, as already discussed in section 6.5. By ”tradition” Walker and Gylling (1998), Gylling et al. (1999a) and Walker and Gylling (1999) present the results as ”travel time”. Furthermore, these ”transit times” are calculated assuming a porosity of 10^{-4}, rather than 10^{-3} as suggested above. However, by noting that $a_w=a_r/\varepsilon$ for constant porosity it is seen that the F-quotient does not depend on porosity. Table 7.3.2 displays the results using the a_r values suggested above. The following may be observed from the table.

- For Aberg most variants are very similar to the base case. The variants without structures are not really physically motivated and could thus be discarded (their deviation from the base case is also relatively minor).

- Also for Beberg most variants are similar to the base case. However, the variant with environmental head has a lower minimum a_rL/q and is thus a candidate for a pessimistic case. It can be noted that the median a_rL/q is lower (but similar) for pathlines leaving the western boundary also these paths need be considered as the remaining fate of the pathlines outside the model domain is unknown. (It is not unlikely that the additional contribution to a_rL/q is small if the remaining transport would occur through a fracture zone).

- For Ceberg most variants are similar to the base case. The variant with additional conductor domains and increased hydraulic conductivity in the conductor domain show a factor of ten lower minimum a_rL/q. This variant is however, quite extreme as it is based on a “what-if” suggestion. The only pessimistic value, which could find support in the data, would be to take the 95% of the base case values.

Table 7.3.2 *Distribution of transport resistance a_rL/q (yr/m in log scale) obtained from detailed scale hydrogeologic analyses (Walker and Gylling, 1998, Gylling et al., 1999a, Walker and Gylling, 1999) assuming a_r=1 m^{-1} for Aberg and Beberg and 0.1 m^{-1} for Ceberg (for other values of a_r the results should be scaled).*

Case	*Median*	*5%*	*95%*
Aberg			
Base case	5.0	3.9	6.4
Upscaling	4.8	3.8	5.9
Anisotropy	5.0	3.8	6.6
No structures	4.6	3.6	5.8
No structures and conditioning	4.5	3.4	5.8
Deterministic –Homogeneous	5.1	4.3	6.0
Beberg			
Base case	5.8	5.0	6.4
Environmental head – top	5.5	4.5	6.2
- Bottom	5.6	4.8	6.3
- Western side	5.2	4.7	7.0
Additional zones	5.7	4.9	6.3
Alt. depth dep. + envin. BC – top	5.9	4.7	6.6
- Bottom	6.3	5.8	6.8
- Vertical sides	5.6	5.0	5.9
Deterministic – Homogeneous	5.4	4.7	5.8
Ceberg[1]			
Base case	6.2	5.6	6.8
Increase K in CD	6.0	5.3	6.6
Additional CD and increased K in CD	5.9	4.7	6.6
Increased variance in both RD and CD	6.1	5.4	6.7
Deterministic – Homogeneous	6.3	5.7	6.8

[1] Only particles leaving the top surface are included in the statistics, see Gylling et al. (1999).

It could also be noted that the a_rL/q of Aberg is almost one orders of magnitude lower than that of Ceberg. The Beberg values are similar, but slightly higher (factor of 4) than the Aberg values. Most of these differences can probably be directly related to the suggested difference in hydraulic conductivity of the sites (see Walker *et al.*, 1997 and table 6.3.1), although counteracted by the factor of ten decrease in a_r suggested for Ceberg.

It is also worthwhile to consider whether other model approaches would result in different results. As already discussed in section 6.5.4 several different modelling exercises of Aberg exist. Table 7.3.3 displays the F-quotients resulting from these different models. It should be understood that the results are not fully comparable, but tentatively it can be seen that most other analyses results are found within the range of the base case of Walker and Gylling (1998). The discrete network analysis (Dershowitz *et al.*, 1999) allows for a direct integration of F along migration paths. Local values of a_r are estimated from fracture intersection lengths in the model. The results are comparable, but show a much wider spread (up to two orders of magnitude, Selroos and Ström, 1999). The value is of course not fully comparable to the other values due to the differences in estimation technique.

Table 7.3.3 *Distribution of transport resistance a_rL/q (years/m in log scale) obtained from different detailed scale hydrogeologic analyses of Aberg.*

Case	*Median*	*5%*	*95%*
Base case (Walker and Gylling, 1998)	5.0	3.9	6.4
HYDRASTAR (Widén and Walker, 1999)	5.5	4.1	6.9
DFN (Dershowitz *et al.*, 1999)[1,2]	5.7	3.9	7.6
CHAN3D (Gylling *et al.*, 1999b)	4.9	3.9	6.3
SKI SITE-94, SKI, 1996[3]	4.8	2.8	6.8

[1] Only 39% of all pathways [2] Results are approximate for "sector 6", table 5-21 in Dershowitz *et al.* (1999). [3] Various approaches.

Based on these observations it seems reasonable to apply the stochastic continuum results of Walker and Gylling (1998), Gylling et al. (1999a) and Walker and Gylling (1999) to derive parameters to FARF31, even if other approaches potentially can provide further insight into the properties of the flow field. In practice, this also means that the transit times estimated can be as input values to FARF31 as long as differences in a_r and porosity are handled by adjusting a_w such that the desired F-values are reached.

In summary the following suggestions seems highly motivated:

- Select the base cases of Aberg, Beberg and Ceberg respectively as the *reasonable estimate*s of the F-quotient (a_rL/q) and the median of these base cases as the best case single value illustration. For Aberg this implies, t_w=10 yr. and $a_w=10^4$ for a logF=5.0, for Beberg this implies t_w=60 yr and $a_w=10^4$ for a logF=5.7 and for Ceberg this implies t_w=1780 yr≈2000 yr and $a_w=10^3$ for a logF=6.2).
- Select the minimum (5%) F reduced by a factor of 10 to account for uncertainty in a_r for; the Aberg base case (i.e. 0.8 yr. and $a_w=10^3$ for a log F=2.9), for the Beberg environmental head variant (3.3 yr. and $a_w=10^3$ for a log F=3.5) and for the Ceberg the base case (i.e. t_w=400 yr. and $a_w=10^3$ for a log F=5.6) as pessimistic values at the different sites.
- Consider the full range spatial variability of the respective base cases for probabilistic analyses (since the most variants are quite similar to the base case).

Peclet number

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.

Correlation

There may be a correlation between hydraulic conductivity, flow wetted area per volume of rock and porosity, but at present the experimental support for including such correlation is too weak. Furthermore, if correlation is introduced it is important not only to limit this to porosity in calculating transit time. The integrated effect on the F-quotient needs to be handled.

The potential correlation between near-field flow and far-field migration parameters has already been discussed in section 7.2.3. The correlation resulting from the hydraulic simulations is taken care of as the near-field darcy velocity and the far-field ”transit time” are sampled from the same canister position.

There is no study on potential correlation between flow related migration parameters and properties of the rock matrix.

Maximum matrix penetration depth

FARF31 also allows for a maximum diffusion penetration distance into the rock matrix. Based on the assertion by Ohlsson and Neretnieks (1997) that the diffusivity values are based on undisturbed rock (see section 5.5) there should not be any physical limit for this diffusion. There is, however, a symmetry limit as the migration could not proceed further than half the distance between two active migration paths. This distance is related to the conductive fracture frequency, and it is suggested to use depth=$2/a_r$, i.e. 2 m for Aberg and Beberg and 20 m for Ceberg. These distances are much longer than the actual penetration of a sorbing nuclide, which usually is at the order of a few cm. The value of the maximum penetration depth is thus not very important.

7.3.4 Quantification of uncertainties

Table 7.3.4 summarises the above recommendations.

Table 7.3.4 *Suggested parameters to FARF31. It should be noted that transit time and a_w are correlated and cannot be changed without considering change in the other parameter.*

Case	Aberg	Beberg	Ceberg
"Transit time"	Yrs	Yrs	yrs
Reasonable estimate single	10	60	2000
Pessimistic	0.8	3.3	400
Probabilistic	Base case table 7.3.2	Base case table 7.3.2	Base case table 7.3.2
a_w	(m^{-1})	(m^{-1})	(m^{-1})
Reasonable estimate	10^4	10^4	10^3
Pessimistic	10^3	10^3	10^3
Probabilistic	10^3-10^5	10^3-10^5	10^3-10^4
Pe			
Reasonable estimate	10	10	10
Pessimistic	2	2	2
Probabilistic	2-50	2-50	2-50
Max penetration	M	m	m
Reasonable estimate	2.0	2.0	20
Pessimistic	0.2	0.2	2.

8 Biosphere

8.1 Source of information

Bergström *et al.* (1999) present the underlying model assumptions for the *biosphere modules*, which are models of essential components of the biosphere to be used in SR 97. The same report also provides, based on a literature survey, the non-site specific input data to these model modules.

Nordlinder and Bergström (1999) applies this model to the SR 97 sites and suggest *ecosystem specific* dose conversion factors (EDF) for different modules at each site to use in consequence analysis. The site specific information is essentially obtained from maps, climatological data and well capacity data from the Swedish Geological Survey (SGU, 1997). Nordlinder and Bergström remark that better site specific data could be obtained if needed in the future. The present data should rather be seen as examples.

8.2 Use in SR 97, modelling approach and conceptual model uncertainties

The purpose of the biosphere modelling in SR 97 is to assess the radiological consequences of radionuclide releases into the biosphere. The biosphere modelling aims at describing the transfer of radionuclides in the biosphere in order to make it possible to estimate radiological consequences for man and the environment from radionuclide releases into the biosphere. A primary endpoint in the modelling is assessing individual doses to exposed groups. The modelling is performed in different steps. Prior to the near- and far-field release calculations each site is first divided into different ecosystem type *modules* and then EDF:s are calculated in such each module. In the final assessment, the BIO42 code in the calculation chain select a module based on the predicted recharge point in the far-field assessment and calculates doses (Sv/yr) by multiplying the release from the far-field (in terms of Bq/yr) with the EDF:s (Sv/Bq) of the selected module.

Bergström *et al.* (1999) describe the radionuclide transfer in the different ecosystem type modules. Nordlinder and Bergström (1999) divide the SR 97 sites into such modules, determine the site specific parameters and calculate EDF:s. The dose calculations will be made as part of the final assessment.

8.2.1 Biosphere modules

In the modelling approach, recipient areas in the biosphere consists of one or several major types of ecosystems modules. Bergström *et al.* (1999) consider the modules: *well,* *lake, running water, coast, soil* and *peat*. There is also an *irrigation* module which is a sub-module in the well, the lake and the running water modules. The module models aim to represent the most important exposure pathways to the exposed group relevant for the module. Due to lack of relevant data, Bergström *et al.* (1999) did not develop a forest ecosystem, but there is nothing in the approach that would not allow such a module. The modules are divided into one or more "compartments" and the ecological situation to be dealt with is described in the form of a "transfer factors" between the compartments. The approach leads to the formulation of a set of differential equations which are solved by the BIOPATH-code (Bergström *et al.*, 1982).

In modelling radionuclide transfer inside a module Bergström *et al.* (1999) acknowledge that man may be exposed both externally and internally from radiation of radionuclides transferred into the biosphere. External exposure may occur from ground deposition or immersion in contaminated air and water. Intake of radionuclides, as well as inhalation leads to internal exposure. The type of ecosystem to which radionuclides enter determines which exposure pathways to consider. Nuclides in compartments like soil, water and sediments may be taken up by living organisms and be further moved along the food chains.

To obtain daily intakes, the concept of most exposed group is used. The most exposed group is defined as a group of people which can be expected to obtain the highest doses from the nuclear facility of concern. It is assumed that all exposed groups are self-sustaining households, leading to pessimistic estimates of their exposure, since self-sustained households are rare in our current society.

The doses to man are obtained by multiplying the intake rates with nuclide specific dose conversion factors, expressed as Sv per Bq ingested/inhaled and by multiplying the soil concentration with dose conversion factors for external radiation in terms of Sv per Bq per m^2 or per kg soil. The factors are taken from the recommendations by the International Commission on Radiation Protection (ICRP 60, 1991) and should not be confused with the EDF:s which also includes the impact of transfer within the biosphere. The dose conversion factors used are listed in table 2.1 in Bergström *et al.* (1999).

Bergström *et al.* (1999) note the following general simplification of the modelling approach:

- Retardation processes in the saturated/unsaturated groundwater flow in the soil are generally not considered as they depend on detailed information on the hydrogeological and migration characteristics of the subsurface. This implies that there is no modelled retardation between the geosphere release point and the module of interest. This assumption will lead to overestimation of consequences of a direct release but can underestimate consequences of accumulation in the upper groundwater flow system.

- Nuclides discharged into a water compartment dissolve homogeneously and immediately, but may then sorb onto particulate matter in the water.

- As with any compartment model, it is assumed to be a homogeneous distribution of radionuclides in the soil- and peat compartments.

- Mean annual values and conditions are assumed for hydrological conditions.

- There is no reduction of the amount of radionuclides in the compartments due to biotic uptake. This is probably a pessimistic assumption as such processes cause a transport of elements out of the area.

- The uptake of nuclides in biota of food chains is described by ”steady-state” linear distribution factors. This assumption may underestimate the effect of accumulation and especially with respect to the aquatic uptake. For example, the true levels of radionuclides in fish result from an integration of uptake over time, whereas the use of a linear distribution factor always will make the fish concentration proportional to the current concentration in the water.

- No evolution of the biosphere is considered. This is in accordance with the suggested radiological criteria suggested by SSI (1998) but could still possibly result in an absurd situation, in particular if EDF:s are to be applied to scenarios, such as glaciation, in the distant future. For the initial defect canister scenario, however, this limitation is of a little less concern.

Bergström *et al.* (1999) note that several complicated interactions are simplified, but often indirectly considered due to the use of empirical data for the transfer of radionuclides within the biosphere. Still, the conceptual model uncertainty relating to the effect of biological accumulation has to be acknowledged. For SR 97, the strong retention of elements considered in the soil and peat module could still be used to illustrate the significance of accumulation.

Doses to organisms other than man are not calculated. However, the modulisation anyway allows for a discussion of consequences in different areas of the repository site. It is generally argued that as long as man is protected there is no real danger for life. This appears to be a relevant assumption since the modelling assumes that man actually uses the biosphere in the compartment. Still some organisms may certainly receive much higher doses that man in a real situation.

8.2.2 Assignment of models to specific ecosystems

In applying the biosphere modules to the SR 97 sites Nordlinder and Bergström (1999) divide each site into sub-areas (250 m x 250 m), associate a specific module to each sub area and then determine the site specific parameters for this sub-area. The module type is selected from present day conditions, mainly from inspection of maps. Well modules occur when the well-archive (SGU, 1997) has a registered well in the area. As there is no forest-type module developed, at present, forest sub-areas are associated with the module type lying ”down-stream” of the area. In cases where there is discussion on which module type to associate with a sub-area, the module type giving rise to the highest dose consequences is selected. (Strictly, this means that the selection could only be made when the far-field radionuclide release is known. In practise this is a problem only when selecting among the peat, soil and well systems, see below).

There is no communication between the modules. A dose *only* occurs in the first module receiving the activity inflow and is then ”forgotten” (i.e. if nuclides discharge into a stream, the running water module will apply, but (a potential) lake module downstream will not be considered). Evidently the model builds on the fact that the HYDRASTAR migration paths will end up in a unique release point for a given realisation and canister position as long as there is a single canister failure. It is assumed that the maximum consequence will occur in the module where the release first enters the biosphere, but this may not be totally true. For example, radionuclides released into a river may sorb on the particulate matter, which in turn may sediment in a delta. The doses in the delta ecosystem may then potentially be higher than in the river system.

The lack of forest modules is also a concern. It is not clear that simple transfer into the downstream module type will produce realistic estimates and it is certainly not pessimistic. In particular, for Aberg where there are many forest areas in direct contact with the sea, this principle leads to that most of the site is associated with coast and open bay (i.e. coast) modules (see figures A.1 and A.2 in Nordlinder and Bergström, 1999). Releases into a coast module will generally result in very low doses due to the large dilution volumes in such a module.

Clearly, the module assignment and the assumptions made that the modules do not communicate implies a risk that the biosphere ”selected” by the migration path may not be the most appropriate one. For the *reasonable estimate* assumptions this may not be a big concern since the far-field release point is an evident first guess. However, if there is need to discuss likelihood, which is needed for the *probabilistic* case, this is a concern.

Given the fact that there are many different options for radionuclide transfer and accumulation in the biosphere it may in fact be very hard to prove absolute conservatism. Instead, the approach has to be to illustrate the significance of these uncertainties by selecting ”pessimistic” parameters in the available models. This approach would imply that in order to account for the uncertainty connected to module communication a pessimistic route would be to always select the module with the highest conversion factors. This approach could also be used to account for uncertainty in release points, even if multiple realisations from HYDRASTAR will provide a fairly good view on this range. It should be noted though, that ”worst” is nuclide specific, as will be further discussed below.

8.3 Data uncertainties, correlations and dependencies on other parameters

8.3.1 Individual modules

The biosphere modules generally include the following three sets of parameters:

- *Biological parameters* (root uptake, uptake to fish, crustacean and aquatic plants, translocation, metabolism in cattle, yield values etc…)
- *Chemical/physical parameters* (volumes, water flows, sorption parameters etc..)
- *Human behaviour* (irrigation, keeping cattle outdoors, consumption patterns etc..)

Of these parameters Bergström *et al.* (1999) only view few to be site specific, as can be seen from Table 8.3.1. The table also displays the dominating pathway in the different modules.

Table 8.3.1: *Site specific data and dominating pathways in the modules modelled by Bergström et al. (1999).*

Module	Site specific data	Dominating pathway
Well	Dilution volume (set equal to the well capacity). (Is set to 2000 m^3/year).	Consumption of water for most nuclides. Milk and meat (from cattle drinking well water) give important contributions for iodine and caesium isotopes.
Lake	Area, max depth, Catchment area and run-off, lake volume, precipitation, sediment depths, water turnover rates.	Consumption of fish and crayfish.
Running water	Volumes, drainage areas, water turnover rates.	Consumption of fish. Drinking water non-negligible for actinides
Coast	Volumes, water depths, water turnover rates	Consumption of fish
Soil	None – except distribution in order to select this as a module	Inhalation for actinides except ^{237}Np, Ni ^{129}I and Cs through milk and meat.
Peat	None – except distribution in order to select this as a module	Milk and meat for ^{129}I. Inhalation for actinides except ^{237}Np

Bergström *et al.* (1999) present (a limited) uncertainty analysis of resulting EDF:s based on release of 1 Bq/yr (of each considered nuclide) during 10 000 years. The ranges of data considered are based on a literature survey. Correlation factors are used in many instances, e.g. between distribution coefficients and root-uptake and between consumption of fish and meat. The actual data used are presented in Appendix A of Bergström *et al.* (1999). The analysis does not fully cover the impact of the dispersion volumes, since these are specific to each site.

Typically the range of uncertainty considered results in a two orders of magnitude uncertainty. Furthermore, Bergström *et al.* (1999) conclude that generally the considered uncertainty in the *biological* parameters contribute the *most* to the uncertainty in resulting dose and the considered uncertainty in *human behaviour* contribute the *least* to the uncertainty in resulting dose. In many studies of this type the main contribution to uncertainty is due to the dispersion volumes applied (BIOMOVS 2, 1996). This uncertainty is here instead, to a large extent, covered by the differences between the modules and by the uncertainty in the site specific parameters (i.e. the dilution volumes). Inspection of the results of the site specific application of the modules presented in Nordlinder and Bergström (1999) shows that the EDF uncertainty within a specific module is far less than differences between modules.

Also the dose conversion factors recommended by ICRP are estimates of the actual impact rather than deterministic predictions. The ICRP recommendations are also subject to continuous revision and some minor adjustments have been made over the years.

8.3.2 Module selection and adoption

A simple analysis of the detailed scale hydrogeologic models (*Walker and Gylling, 1998, Gylling et al., 1999a, Walker and Gylling, 1999*) is to select the module directly above the HYDRASTAR path line exit points, and thereby not considering any horizontal transport in the surficial parts of the geosphere. Table 8.3.2 (Kautsky, pers. com) displays the proportion of exit points in different modules calculated in this ways, for the base case of Aberg, Beberg and Ceberg respectively.

Table 8.3.2 *Proportion of exit points in different modules for the Base Case local scale hydrogeological model*

Module	***Proportion of exit points in different modules***		
	Aberg	***Beberg***	***Ceberg***
Forest	18.5	63.7	42.2
Bog	2.5	11.5	26.3
Agricultural land	0.0	24.8	31.4
Lake	0.0	0.0	0.0
Stream	0.0	0.0	0.1
River	0.0	0.0	0.0
Well	0.0	0.0	0.2
Coast (bay)	79.8	0.0	0.0
Coast (open)	0.0	0.0	0.0

The module selection has a great impact on the resulting EDFs. Nordlinder and Bergström (1999) select and adopt the biosphere modules to the SR 97 sites.

Inspection of their results shows that in general, the well, the soil and the peat module result in the highest equivalent dose conversion factors. These modules have far less dilution, than the lake, stream or open coast modules.

Nordlinder and Bergström (1999) note that the present site specific input data is basically confined to information available from maps and suggest that more refined information could be obtained in a future update of the models. However, such increased precision is possibly of limited value given the large difference between EDFs for different module types, the lack of a proper model for bio-accumulation, the lack of a forest module and the uncertainty in transition between modules. It should also be remembered that the actual discharge points of radionuclides released into the geosphere are quite uncertain. Even if this uncertainty to a large extent is covered by different HYDRASTAR variants combined with the uncertainty in the position of the initially damaged canisters, the net result is true uncertainty (although within limits) on where, if ever, radionuclides released from a single failed canister will enter the biosphere. Given these uncertainties it does not seem reasonable to put too much emphasis on the release positions. As already discussed, however, the main uncertainty in the analysis is the validity of the conceptual model.

8.3.3 Quantification of uncertainties

In light of the discussion in previous sections the following is suggested for application on SR 97: For a *reasonable estimate* one should use the mean values of the EDFs and select the module according to the geosphere reasonable estimate release point(s). In accordance with section 6.5 and chapter 7 it is thus suggested to select the release points predicted by the base case of Walker and Gylling (1998), Gylling et al. (1999a) and Walker and Gylling (1999) for Aberg, Beberg and Ceberg respectively as reasonable estimate. As can be seen from table 8.3.2, 79% of the streamtubes discharge into the inner bays of Aberg ("archipelago"). In fact, also most streamtubes classified as "forest" or "peat" ("bog") could be classified as "archipelago" since they discharge very close to the shore line. Consequently, the inner bay of Aberg is the reasonable estimate module for Aberg. In Beberg "forest" is the most common exit point (64%), but in the modelling all forest parts are treated as "peat" since, at present, there is no forest module in the model. In Ceberg, the proportions of "forest", "peat bog" and "agricultural" are all quite high (42%, 26% and 31% respectively). However, since forest and peat are brought together, peat is the most common module and should thus be treated as a reasonable estimate. Still, also peat is potentially possible at Aberg, so also the peat module needs to be assessed. Furthermore, at all sites it seems motivated to apply a standard well (300 l/min capacity), in order to simplify comparison of the releases at the three different sites.

For a *pessimistic case* one should use extreme values of the EDFs, apply the well, peat and soil module and select the MODULE resulting in the highest doses. In addition it will be necessary to discuss implications of bio-accumulation.

For *probabilistic* analyses one should pick the modules implied by the discharge points from the flow solution of Walker and Gylling (1998), Gylling et al. (1999a) and Walker and Gylling (1999). The specific choices are already discussed in chapter 7.

Table 8.3.3 summarises these recommendations.

Table 8.3.3: *Suggested quantification of uncertainties in biosphere module*

Case	**Aberg**	**Beberg**	**Ceberg**
Module			
Reasonable estimate single	Inner bay of Aberg (but compare with well and peat)	Peat (but compare with well)	Peat (but compare with well)
Pessimistic	Apply the well, peat and soil module select the MODULE resulting in the highest dose. Discuss implications of bioaccumulation.	Apply the well, peat and soil module select the MODULE resulting in the highest dose. Discuss implications of bioaccumulation.	Apply the well, peat and soil module select the MODULE resulting in the highest dose. Discuss implications of bioaccumulation.
Probabilistic	Select the module consistent with discharge in Aberg flow case Walker and Gylling (1998) selected for probabilistic assessment.	Select the module consistent with discharge in Beberg flow case Gylling *et al.* (1999a) selected for probabilistic assessment.	Select the module consistent with discharge in Ceberg flow case Walker and Gylling (1999) selected for probabilistic assessment.
EDF for selected modules			
Reasonable estimate	Median values	Median values	Median values
Pessimistic	Maximum values	Maximum values	Maximum values

9 Conclusions

The present report:

- establishes a framework for handling data uncertainty within SR 97,
- explores uncertainties in the different underlying analyses which provide input to the radionuclide release and transport models used to explore the radiological consequences of the SR 97 canister defect scenario,
- suggests and motivates ”reasonable estimate” input values, and ”pessimistic” input values representing, when applicable, conditions at Aberg, Beberg and Ceberg, for the different models used,
- suggests ”probabilistic distributions” for the parameters where such distributions can be motivated.

The uncertainly evaluation concentrates on the quantitative models or analyses actually selected for the model chain. The issue of conceptual model uncertainty is partly included in this evaluation, whereas the more fundamental questions concerning model selection and which potential model couplings to analyse are not addressed here but in the SR 97 report directly or in underlying reports of the SR 97 report.

Even if is has been possible to meet the objectives of the work it is inevitable that the quality of the estimates varies for the different explored analyses. Sometimes the reasonable estimate parameters are well founded on a solid experimental or theoretical basis and sometimes they just represent median values on a very wide and uncertain distribution. Some of the pessimistic values are realistic estimates of the worst possible conditions, whereas others are selected solely to be defensible. Furthermore, it is only at rare occasions where it is possible to estimate sharper probabilistic uncertainty distributions than a parameter range. Still an effort has been made to explore correlations between processes and parameters such that unrealistic combinations of parameter values would not be analysed.

It is possible that further efforts would make it possible to provide more sharp uncertainty estimates. However, judging from the state of information as presented in this report such efforts should only be directed into areas where a the impact would be significant. Prime candidates for such increased efforts would be parameters where the impact resulting from reasonable estimate parameter values and from pessimistic values is large.

Finally, it should be noted that the present report does not discuss how to select combinations of parameters. This selection is discussed in the main SR 97 report.

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Appendix A

A:1 Spent fuel and canister data

A:1.1 Inventory

Table A.1.1.1: *Suggested quantification of uncertainty in inventory*

Case	Description
Reasonable estimate	Inventory estimated by Håkansson (1998) for 12 BWR 38 MWd/kg U after 40 years (i.e. table 9).in Håkansson (1998) and table A.1.1.2.
Pessimistic case	Not applicable.
Uncertainties	Qualitative evaluation of the impact on release from COMP23 due to i) effect of PWR canisters ii) effect of higher burn-up composition iii) uncertainty suggested by Håkansson (1997) while still considering constant initial heat load

Table A.1.1.2: *Inventory for BWR 38 MWd/kg U after 40 years(taken from table 9 of Håkansson, 1998).*

Nuclide	Activity (Bq/t U) 40 years after discharge	Nuclide	Activity (Bq/t U) 40 years after discharge	Nuclide	Activity (Bq/t U) 40 years after discharge
Fission products		*Actinides*		*Light elements*	
H-3	$2.1\cdot10^{12}$	Ra-226	$1.4\cdot10^{5}$	H-3	$1.1\cdot10^{12}$
Se-79	$2.8\cdot10^{9}$	Th-229	$1.0\cdot10^{4}$	C-14	$5.0\cdot10^{10}$
Kr-85	$2.7\cdot10^{13}$	Th-230	$1.6\cdot10^{7}$	Cl-36	$5.5\cdot10^{8}$
Sr-90	$1.2\cdot10^{15}$	Th-234	$1.2\cdot10^{10}$	Fe-55	$9.3\cdot10^{9}$
Y-90	$1.2\cdot10^{15}$	Pa-231	$1.8\cdot10^{6}$	Co-60	$8.9\cdot10^{11}$
Zr-93	$5.0\cdot10^{10}$	Pa-233	$1.5\cdot10^{10}$	Ni-59	$8.8\cdot10^{10}$
Nb-93m	$4.2\cdot10^{10}$	Pa-234m	$1.2\cdot10^{10}$	Ni-63	$9.3\cdot10^{12}$
Tc-99	$5.7\cdot10^{11}$	U-233	$3.1\cdot10^{6}$	Sr-90	$2.6\cdot10^{7}$
Ru-106	$2.7\cdot10^{4}$	U-234	$4.6\cdot10^{10}$	Y-90	$2.6\cdot10^{7}$
Pd-107	$4.9\cdot10^{9}$	U-235	$4.5\cdot10^{8}$	Zr-93	$5.6\cdot10^{9}$
Cd-113m	$1.7\cdot10^{11}$	U-236	$1.0\cdot10^{10}$	Nb-93m	$2.3\cdot10^{10}$
Sn-121	$4.4\cdot10^{10}$	U-237	$1.9\cdot10^{10}$	Nb-94	$2.9\cdot10^{9}$
Sn-121m	$5.7\cdot10^{10}$	U-238	$1.2\cdot10^{10}$	Mo-93	$4.4\cdot10^{7}$
Sb-125	$1.1\cdot10^{10}$	Np-237	$1.5\cdot10^{10}$	Ag-108	$4.3\cdot10^{7}$
Te-125m	$2.7\cdot10^{9}$	Np-239	$1.2\cdot10^{12}$	Ag-108m	$5.0\cdot10^{8}$
Sn-126	$2.3\cdot10^{10}$	Pu-238	$9.5\cdot10^{13}$	Cd-113m	$3.4\cdot10^{10}$
Sb-126m	$2.3\cdot10^{10}$	Pu-239	$9.5\cdot10^{12}$	Sn-121	$1.4\cdot10^{10}$
I-129	$1.3\cdot10^{9}$	Pu-240	$1.2\cdot10^{13}$	Sn-121m	$1.7\cdot10^{10}$
Cs-134	$9.1\cdot10^{9}$	Pu-241	$7.7\cdot10^{14}$	Sb-125	$1.2\cdot10^{9}$
Cs-135	$2.1\cdot10^{10}$	Pu-242	$1.0\cdot10^{11}$	Te-125m	$3.0\cdot10^{8}$
Cs-137	$1.8\cdot10^{15}$	Am-241	$1.5\cdot10^{14}$	Eu-154	$3.2\cdot10^{11}$
Ba-137m	$1.7\cdot10^{15}$	Am-242m	$4.5\cdot10^{11}$	Eu-155	$1.3\cdot10^{10}$
Pm-146	$9.8\cdot10^{8}$	Am-242	$4.5\cdot10^{11}$	Ho-166m	$7.5\cdot10^{7}$
Pm-147	$1.5\cdot10^{11}$	Am-243	$1.2\cdot10^{12}$	*Total*	$1.2\cdot10^{13}$
Sm-151	$9.4\cdot10^{12}$	Cm-242	$3.7\cdot10^{11}$		
Eu1-52	$3.3\cdot10^{10}$	Cm-243	$4.4\cdot10^{11}$		
Eu-154	$1.8\cdot10^{13}$	Cm-244	$2.8\cdot10^{13}$		
Eu-155	$7.6\cdot10^{11}$	Cm245	$9.4\cdot10^{9}$		
Total	$6.0\cdot10^{15}$	Cm-246	$2.9\cdot10^{9}$		
		Total	$1.1\cdot10^{15}$		

A:1.2 Radionuclide release from the spent fuel

Table A.1.2.1: *Suggested quantification of uncertainties in fuel conversion*

Case	Description
Reasonable estimate	Constant dissolution rate 10^{-8} yr^{-1}
Pessimistic case	Not meaningful – discuss implications of uncertainty in safety assessment

Table A.1.2.2: *Suggested quantification of uncertainties in IRF*

Case	Description
Reasonable estimate	Use reasonable estimate (including metal parts) in table A.1.2.3
Pessimistic case	Use pessimistic estimate in table A1.2.3

Table A.1.2.3: *Reasonable estimate and pessimistic IRF values for some key nuclides, taken from table 3 in Johnson and Tait (1997) and complemented with assumptions concerning the metal parts.*

Nuclide	***IRF(%) reasonable estimate - only fuel***	***IRF(%) reasonable estimate including metal parts***	***IRF(%) pessimistic estimate***
C-14	5	15	55
Cl-36	6	6	12
Co-60	-	-	-
Ni-59	-	100	100
Ni-63	-	100	100
Se-79	3	3	6
Kr-85	2	2	4
Sr-90	0.25	0.25	1
Zr-93	-	-	-
Nb-94	-	100	100
Tc-99	0.2	0.2	1
Pd-107	0.2	0.2	1
Ag-108m	3	100	100
Cd-113m	3	3	6
Sn-126	2	2	4
I-129	3	3	6
Cs-135	3	3	6
Cs-137	3	3	6
Sm-151	-	-	-
Eu-154	-	-	-
Ho-166m	-	-	-
actinides	-	-	-

A:1.3 Canister defects, delay time and defect growth

Table A.1.3.1: *Suggested quantification of uncertainties in canister defect, delay time and defect growth*

Case	Initial defect	Growth	Delay time
"Reasonable estimate"	1 canister with 1 mm^2 (1 μm thin and 1 m long) defect	Complete failure, i.e. a failure large enough (1 dm^2) not to offer any migration resistance after $2 \cdot 10^5$ years	$2 \cdot 10^5$ years
Pessimistic	5 canisters with the 1 mm^2 (1 μm thin and 1 m long) defect	Complete failure, i.e. a failure large enough not to offer any migration resistance, after $2 \cdot 10^4$ yrs	300 yrs
Probabilistic	A number uniformly distributed in the range 1 to 5 canisters (0.1 % of all) having a 1 mm^2 (1 μm thin a 1 m long(defect.	Complete failure, i.e. a failure large enough not to offer any migration resistance, distributed between $2 \cdot 10^4$ yrs - $2 \cdot 10^5$ yrs	between 300 years and time at complete failure
Variants	Failure in bottom	n.a.	"The water exclusion case" according to Bond *et al*. (1997).

A:2 Chemical and Physical Data

A:2.1 Groundwater chemistry

Table A.2.1.1: *Suggested quantification of uncertainty in water chemistry*

Case	**Aberg**	**Beberg**	**Ceberg**
Reasonable estimate	Reference water for Aberg in Laaksoharju *et al*., 1997, but consideration of different buffer pore water (see section 5.2 and 5.3)	Reference water for Beberg (KFI07) in Laaksoharju *et al*., 1997, but consideration of different buffer pore water (see section 5.2 and 5.3)	Reference water for Ceberg in Laaksoharju *et al*., 1997, but consideration of different buffer pore water (see section 5.2 and 5.3)
Pessimistic	Select the water chemistry in the range of reference waters in Laaksoharju *et al*. (1997) and buffer pore water, which will produce the most pessimistic solubility, diffusivity or sorption coefficients.	Select the water chemistry in the range of reference waters in Laaksoharju *et al*. (1997) and buffer pore water, which will produce the most pessimistic solubility, diffusivity or sorption coefficients.	Select the water chemistry in the range of reference waters in Laaksoharju *et al*. (1997) and buffer pore water, which will produce the most pessimistic solubility, diffusivity or sorption coefficients.

A:2.2 Solubilities

Table A.2.2.1: *Suggested quantification of uncertainty in solubility*

Case	Aberg	Beberg	Ceberg
Reasonable estimate	See table A.2.2.3. The highest of the Aberg solubility and the bentonite solubility of table A.2.2.2 Table A2.2.2 is based on the highest for Äspö (Aberg) in table 9-4 in Bruno *et al.* (1997).	See table A.2.2.3. The highest of the Beberg solubility and the bentonite solubility of table A2.2.2 Table A.2.2.2 is based on the highest for Finnsjön (Beberg) in table 9-4 in Bruno *et al.* (1997).	See table A.6.3. The highest of the Ceberg solubility and the bentonite solubility of table A.2.2.2 Table A.2.2.2 is based on the highest for Gideå (Ceberg) in table 9-4 in Bruno *et al.* (1997).
Pessimistic	See table A.2.2.3 (based on the highest for each element in table 7-4 (bentonite), table 9-4 and table 11-7 in Bruno *et al.* (1997).	See table A.2.2.3 (based on the highest for each element in table 7-4 (bentonite), table 9-4 and table 11-7 in Bruno *et al.* (1997).	See table A.2.2.3 (based on the highest for each element in table 7-4 (bentonite), table 9-4 and table 11-7 in Bruno *et al.* (1997).

Table A.2.2.2 *Solubilities (in mole/dm^3) for the species resulting in the highest solubilities as calculated by Bruno et al. (1997.)*

Element	**Aberg**	**Beberg**	**Ceberg**	**Bentonite**	**Range**	**Pessimistic**
pH	7.70	7.90	9.30	9.21	table 11-7 in Bruno	maximum
pe	-5.21	-4.23	-3.41	-6.51	*et al.* (1997)	value
Ni	$5.15 \cdot 10^{-6}$	$9.73 \cdot 10^{-6}$	$2.07 \cdot 10^{-8}$	high	$1 \cdot 10^{-5}$-$1 \cdot 10^{-1}$	high
Se	$7.34 \cdot 10^{-10}$	$3.52 \cdot 10^{-11}$	$9.80 \cdot 10^{-12}$	$2.59 \cdot 10^{-9}$	$4 \cdot 10^{-11}$-$4 \cdot 10^{-9}$	high
Sr	$6.88 \cdot 10^{-3}$	$3.09 \cdot 10^{-3}$	$3.05 \cdot 10^{-5}$	$1.21 \cdot 10^{-4}$	$6 \cdot 10^{-7}$-$4 \cdot 10^{-2}$	$4 \cdot 10^{-2}$
Zr	$2.48 \cdot 10^{-9}$	$2.51 \cdot 10^{-9}$	$2.51 \cdot 10^{-9}$	$2.50 \cdot 10^{-9}$	$2 \cdot 10^{-9}$-$3 \cdot 10^{-9}$	$3 \cdot 10^{-9}$
Nb	$6.08 \cdot 10^{-5}$	$7.44 \cdot 10^{-5}$	$1.39 \cdot 10^{-3}$	$1.37 \cdot 10^{-3}$	$2 \cdot 10^{-5}$-$4 \cdot 10^{-2}$	$4 \cdot 10^{-2}$
Tc	$7.14 \cdot 10^{-9}$	$7.92 \cdot 10^{-9}$	$7.27 \cdot 10^{-9}$	$7.67 \cdot 10^{-9}$	$4 \cdot 10^{-9}$-$5 \cdot 10^{-8}$	$5 \cdot 10^{-8}$
Pd	$4.21 \cdot 10^{-9}$	$4.17 \cdot 10^{-9}$	$4.18 \cdot 10^{-9}$	$4.17 \cdot 10^{-9}$	$4 \cdot 10^{-9}$-$8 \cdot 10^{-9}$	$8 \cdot 10^{-9}$
Ag	$2.96 \cdot 10^{-5}$	$9.39 \cdot 10^{-7}$	$7.12 \cdot 10^{-7}$	$4.64 \cdot 10^{-20}$	$3 \cdot 10^{-5}$-$3 \cdot 10^{-5}$	$3 \cdot 10^{-5}$
Sn	$5.52 \cdot 10^{-10}$	$6.03 \cdot 10^{-10}$	$4.68 \cdot 10^{-9}$	$4.49 \cdot 10^{-9}$	$1 \cdot 10^{-10}$-$1 \cdot 10^{-5}$	$1 \cdot 10^{-5}$
Sm	$2.13 \cdot 10^{-6}$	$2.69 \cdot 10^{-7}$	$2.91 \cdot 10^{-7}$	$8.03 \cdot 10^{-7}$	$3 \cdot 10^{-7}$-$2 \cdot 10^{-5}$	$2 \cdot 10^{-5}$
Ho	$6.27 \cdot 10^{-6}$	$1.52 \cdot 10^{-6}$	$1.97 \cdot 10^{-6}$	$5.58 \cdot 10^{-6}$	$2 \cdot 10^{-6}$-$6 \cdot 10^{-5}$	$6 \cdot 10^{-5}$
Ra	$2.86 \cdot 10^{-7}$	$5.02 \cdot 10^{-7}$	$1.20 \cdot 10^{-4}$	$4.57 \cdot 10^{-8}$	$2 \cdot 10^{-7}$-$2 \cdot 10^{-6}$	$2 \cdot 10^{-4}$
Th	$2.40 \cdot 10^{-10}$	$1.17 \cdot 10^{-9}$	$2.40 \cdot 10^{-10}$	$1.22 \cdot 10^{-9}$	$2 \cdot 10^{-10}$-$5 \cdot 10^{-10}$	$2 \cdot 10^{-9}$
Pa	$3.16 \cdot 10^{-7}$	$3.16 \cdot 10^{-7}$	$3.16 \cdot 10^{-7}$	$3.16 \cdot 10^{-7}$	$3 \cdot 10^{-7}$-$3 \cdot 10^{-7}$	$4 \cdot 10^{-7}$
U	$1.27 \cdot 10^{-7}$	$1.29 \cdot 10^{-7}$	$1.29 \cdot 10^{-7}$	$1.28 \cdot 10^{-7}$	$2 \cdot 10^{-8}$-$2 \cdot 10^{-7}$	$2 \cdot 10^{-7}$
Np	$7.00 \cdot 10^{-9}$	$1.05 \cdot 10^{-7}$	$8.39 \cdot 10^{-9}$	$5.87 \cdot 10^{-8}$	$5 \cdot 10^{-9}$-$6 \cdot 10^{-8}$	$2 \cdot 10^{-7}$
Pu	$6.56 \cdot 10^{-9}$	$5.35 \cdot 10^{-10}$	$1.03 \cdot 10^{-10}$	$1.38 \cdot 10^{-10}$	$1 \cdot 10^{-10}$-$3 \cdot 10^{-6}$	$3 \cdot 10^{-6}$
Am	$6.87 \cdot 10^{-7}$	$9.36 \cdot 10^{-8}$	$4.89 \cdot 10^{-8}$	$9.34 \cdot 10^{-8}$	$1 \cdot 10^{-7}$-$7 \cdot 10^{-6}$	$7 \cdot 10^{-6}$
Cm	$2.22 \cdot 10^{-7}$	$2.02 \cdot 10^{-9}$	$9.01 \cdot 10^{-10}$	$1.66 \cdot 10^{-10}$	$1 \cdot 10^{-11}$-$2 \cdot 10^{-6}$	$2 \cdot 10^{-6}$

Table A.2.2.3 *Reasonable estimate and pessimistic solubilities suggested.*

Element	**Aberg** Best Est.	**Beberg** Best Est.	**Ceberg** Best Est.	**All sites** Pessimistic
Ni	high	high	high	high
Se	$2.59\cdot10^{-9}$	$2.59\cdot10^{-9}$	$2.59\cdot10^{-9}$	high
Sr	$6.88\cdot10^{-3}$	$3.09\cdot10^{-3}$	$1.21\cdot10^{-4}$	$4\cdot10^{-2}$
Zr	$2.50\cdot10^{-9}$	$2.51\cdot10^{-9}$	$2.51\cdot10^{-9}$	$3\cdot10^{-9}$
Nb	$1.37\cdot10^{-3}$	$1.37\cdot10^{-3}$	$1.39\cdot10^{-3}$	$4\cdot10^{-2}$
Tc	$7.67\cdot10^{-9}$	$7.92\cdot10^{-9}$	$7.67\cdot10^{-9}$	$5\cdot10^{-8}$
Pd	$4.21\cdot10^{-9}$	$4.17\cdot10^{-9}$	$4.18\cdot10^{-9}$	$8\cdot10^{-9}$
Ag	$2.96\cdot10^{-5}$	$9.39\cdot10^{-7}$	$7.12\cdot10^{-7}$	$3\cdot10^{-5}$
Sn	$4.49\cdot10^{-9}$	$4.49\cdot10^{-9}$	$4.68\cdot10^{-9}$	$1\cdot10^{-5}$
Sm	$2.13\cdot10^{-6}$	$8.03\cdot10^{-7}$	$8.03\cdot10^{-7}$	$2\cdot10^{-5}$
Ho	$6.27\cdot10^{-6}$	$5.58\cdot10^{-6}$	$5.58\cdot10^{-6}$	$6\cdot10^{-5}$
Ra	$2.86\cdot10^{-7}$	$5.02\cdot10^{-7}$	$1.20\cdot10^{-4}$	$2\cdot10^{-4}$
Th	$1.22\cdot10^{-9}$	$1.22\cdot10^{-9}$	$1.22\cdot10^{-9}$	$2\cdot10^{-9}$
Pa	$3.16\cdot10^{-7}$	$3.16\cdot10^{-7}$	$3.16\cdot10^{-7}$	$4\cdot10^{-7}$
U	$1.28\cdot10^{-7}$	$1.29\cdot10^{-7}$	$1.29\cdot10^{-7}$	$2\cdot10^{-7}$
Np	$5.87\cdot10^{-8}$	$1.05\cdot10^{-7}$	$5.87\cdot10^{-8}$	$2\cdot10^{-7}$
Pu	$6.56\cdot10^{-9}$	$5.35\cdot10^{-10}$	$1.38\cdot10^{-10}$	$3\cdot10^{-6}$
Am	$6.87\cdot10^{-7}$	$9.36\cdot10^{-8}$	$9.34\cdot10^{-8}$	$7\cdot10^{-6}$
Cm	$2.22\cdot10^{-7}$	$2.02\cdot10^{-9}$	$9.01\cdot10^{-10}$	$2\cdot10^{-6}$

A:2.3 Buffer migration data

Table A..2.3.1 *Suggested quantification of uncertainty in buffer migration data*

Case	Description
Reasonable estimate	See table A.2.3.2 (based on reasonable estimate values for saline and reducing in table A.2.3.3)
Pessimistic	See table A.7.2 (based on pessimistic values for saline and reducing in table A.2.3.3)

Table A.2.3.2 *Buffer retention parameters to be used for the canister defect scenario. For further explanation of the use of the table see table A.2.3.1.*

Element	K_d [m^3/kg]		(D_e) [m^2/s]	ε	ρ (kg/m^3)
	Realistic	Pessimistic			
C*	0	0	$3 \cdot 10^{-11}$	0.41	2000
Cl*	0	0	$1 \cdot 10^{-12}$	0.05 (ion excl)	2000
Ni	0.1	0.02	$1 \cdot 10^{-9}$	0.41	2000
Se	0.003	0	$7 \cdot 10^{-11}$	0.41	2000
Sr	0.01	0.001	$5 \cdot 10^{-10}$	0.41	2000
Zr	2	0.05	$5 \cdot 10^{-11}$	0.41	2000
Nb	0.2	0	$5 \cdot 10^{-10}$	0.41	2000
Tc*	0.1	0.01	$5 \cdot 10^{-10}$	0.41	2000
Pd	0.01	0	$1 \cdot 10^{-10}$	0.41	2000
Ag	0	0	$2 \cdot 10^{-10}$	0.41	2000
Sn	3	0.01	$7 \cdot 10^{-11}$	0.41	2000
I*	0	0	$3 \cdot 10^{-12}$	0.05 (ion excl)	2000
Cs	0.05	0.005	$6 \cdot 10^{-10}$	0.41	2000
Ce	1	0.2	$2 \cdot 10^{-10}$	0.41	2000
Sm	1	0.2	$2 \cdot 10^{-10}$	0.41	2000
Ho	1	0.2	$2 \cdot 10^{-10}$	0.41	2000
Pb	0.5	0	$1 \cdot 10^{-9}$	0.41	2000
Rn	0	0	$3 \cdot 10^{-11}$	0.41	2000
Ra	0.01	0.001	$5 \cdot 10^{-10}$	0.41	2000
Th	3	0.1	$7 \cdot 10^{-11}$	0.41	2000
Pa	0.3	0.001	$7 \cdot 10^{-10}$	0.41	2000
U	1	0.01	$5 \cdot 10^{-10}$	0.41	2000
Np	3	0.1	$1 \cdot 10^{-9}$	0.41	2000
Pu	3	1	$3 \cdot 10^{-10}$	0.41	2000
Am	3	1	$7 \cdot 10^{-11}$	0.41	2000
Cm	3	1	$7 \cdot 10^{-11}$	0.41	2000

Table A.2.3.3 *Bentonite migration data suggested by Yu and Neretnieks (1997) and adjusted values suggested by Ochs (1997). For the suggested use of these data, see tables A.2.3.1 and A.2.3.2 above.*

Element	K_d [m^3/kg]		D_a [m^2/s] $D_e/(\varepsilon+k_d\rho)$	(D_e) [m^2/s]	ε	Comments from Ochs	K_d	K_d	D_e
	Realistic	*Pessimistic*	*Realistic*				*Real*	*Cons*	
Am	3	1	$1\cdot10^{-14}$	$7\cdot10^{-11}$		OK			
C^*	0	0	$5\cdot10\cdot^{-12}$	$1\cdot10^{-12}$		OK, but D_a for methane (use Rn data)			PS $3\cdot10^{-11}$
Ce	1	0.2	$1\cdot10^{-13}$	$2\cdot10^{-10}$		OK			
Cl^*	0	0	$2\cdot10^{-11}$	$1\cdot10^{-12}$	0.05	OK, need higher D for elevated T			no
Cs	0.5 (fresh) 0.05 (saline)	0.2 (fresh) 0.005 (saline)	$5\cdot10^{-12}$ $5\cdot10^{-12}$	$6\cdot10^{-9}$ $6\cdot10^{-10}$		fresh K_d:s too high and not relevant			
I^*	0	0	$5\cdot10^{-11}$	$3\cdot10^{-12}$	0.05	Need pessimistic D_e for elevated T			no
Nb	0.2	0	$1\cdot10^{-12}$	$5\cdot10^{-10}$		OK			
Ni	0.1	0.02	$5\cdot10^{-12}$	$1\cdot10^{-9}$		OK			
Np	0.02 (ox) 3 (red)	0.005 (ox) 0.1 (red)	$1\cdot10^{-12}$ $2\cdot10^{-13}$	$5\cdot10^{-11}$ $1\cdot10^{-9}$		A somewhat lower K_d value should be selected for red, to be consistent with D_a	no	no	
Pa	3 (fresh) 0.3 (saline)	0.1 (fresh) 0.01 (saline)	$1\cdot10^{-12}$	$7\cdot10^{-9}$ $7\cdot10^{-10}$		Fresh data irrelevant Uncertainty in redox would motivate K_d=0.001 as a pessimistic limit		0.001	
Pb	0.5	0	$1\cdot10^{-12}$	$1\cdot10^{-9}$		K_d needs to be lower below pH=7. Otherwise reasonable			
Pd	0.01	0	$5\cdot10^{-12}$	$1\cdot10^{-10}$		OK, probably pessimistic. Worthwhile to conduct further studies			
Pu	3	1	$5\cdot10^{-14}$	$3\cdot10^{-10}$		Also include oxidising values K_d= 0.005-0.01 and higher D_a	ox 0.01	ox 0.005	
Ra	0.5 (fresh) 0.01 (saline)	0.1 (fresh) 0.001 (saline)	$2\cdot10^{-11}$ $2\cdot10^{-11}$	2·10-8 $5\cdot10^{-10}$		fresh not relevant saline OK			
Rn	0	0	$1\cdot10^{-10}$	$3\cdot10^{-11}$		OK			
Se	0.003	0	$1\cdot10^{-11}$	$7\cdot10^{-11}$		OK			
Sm	1	0.2	$1\cdot10^{-13}$	$2\cdot10^{-10}$		OK			
Sn	3	0.01	$1\cdot10^{-14}$	$7\cdot10^{-11}$		OK			
Sr	0.5 (fresh) 0.01 (saline)	0.1 (fresh) 0.001 (saline)	$2\cdot10^{-11}$ $2\cdot10^{-11}$	$2\cdot10^{-8}$ $5\cdot10^{-10}$		fresh not relevant saline OK			
Tc^*	0 (ox) 0.1 (red)	0 (ox) 0.01 (red)	$2\cdot10^{-12}$ $2\cdot10^{-12}$	$1\cdot10^{-13}$ $5\cdot10^{-10}$	0.05 (ox)	reducing data OK oxidising Da not consistent			no
Th	3	0.1	$1\cdot10^{-14}$	$7\cdot10^{-11}$		OK			
U	0.05 (ox) 1 (red)	0.005 (ox) 0.01 (red)	$1\cdot10^{-12}$ $2\cdot10^{-13}$	$1\cdot10^{-10}$ $5\cdot10^{-10}$		OK			
Zr	2	0.2	$1\cdot10^{-14}$	$5\cdot10^{-11}$		lower pessimistic K_d to 0.05		0.05	

A:2.4 Backfill sorption and diffusivities

Table A.2.4.1: *Suggested quantification of uncertainties in backfill sorption and diffusivities*

Case	Aberg	Beberg	Ceberg
Reasonable estimate	D_e 10^{-10} m^2/s, saline K_d from Table A.2.4.2 $\varepsilon = 0.30$	D_e 10^{-10} m^2/s, fresh K_d from Table A.2.4.2 $\varepsilon = 0.30$	D_e 10^{-10} m^2/s, fresh K_d from Table A.2.4.2 $\varepsilon = 0.30$
Pessimistic	D_e 10^{-10} m^2/s K_d from Table A.2.4.2, pessimistic, saline $\varepsilon = 0.30$	D_e 10^{-10} m^2/s K_d from Table A.2.4.2, pessimistic, saline $\varepsilon = 0.30$	D_e 10^{-10} m^2/s K_d from Table A.2.4.2, pessimistic saline. $\varepsilon = 0.30$

Table A.2.4.2: *Backfill sorption parameters to be used for the canister defect scenario. Based on proportional contribution from 15% bentonite and 85% crushed rock. Bentonite values are based on Yu and Neretnieks (1997). Rock values are taken from Carbol and Engkvist (1997).*

Element	K_d [m^3/kg]			
	Realistic (saline)	*Realistic (fresh)*	*Pessimistic (saline)*	*Pessimistic (fresh)*
C*	0.0009	0.0009	0.0004	0.0004
Cl*	0	0	0	0
Ni	0.03	0.1	0.01	0.05
Se	0.001	0.001	0.0004	0.0004
Sr	0.002	0.08	0.0002	0.02
Zr	1	1	0.5	0.5
Nb	0.9	0.9	0.4	0.4
Tc*	0.9	0.9	0.3	0.3
Pd	0.01	0.09	0.0009	0.009
Ag	0.05	0.5	0.009	0.1
Sn	0.5	0.5	0.002	0.002
I*	0	0	0	0
Cs	0.05	0.5	0.009	0.1
Sm	2	2	0.9	0.9
Ho	2	2	0.9	0.9
Ra	0.02	0.2	0.009	0.06
Th	5	5	0.9	0.9
Pa	0.9	1	0.4	0.4
U	4	4	0.9	0.9
Np	5	5	0.9	0.9
Pu	5	5	1	1
Am	3	3	1	1
Cm	3	3	1	1

A:2.5 Rock diffusivities

Table A.2.5.1: *Suggested quantification of uncertainties in matrix porosity and rock matrix diffusivities (D_e)*

Case	**Aberg**	**Beberg**	**Ceberg**
Matrix porosity			
All cases	$5 \cdot 10^{-3}$ for all	$5 \cdot 10^{-4}$, for Br, C, Cl, I, $5 \cdot 10^{-3}$ for all others	$5 \cdot 10^{-4}$, for Br, C, Cl, I, $5 \cdot 10^{-3}$ for all others
Diffusivity			
Reasonable estimate	Saline in table A.2.5.2 (based on table 2 in Ohlsson and Neretnieks (1997), for high ionic strength).	Fresh in table A.2.5.2 (based on table 2 in Ohlsson and Neretnieks (1997), for low ionic strength).	Fresh in table A.2.5.2 (based on table 2 in Ohlsson and Neretnieks (1997), for low ionic strength).
Pessimistic	Pessimistic in table A.2.5.2 (Surface diffusion increase is discarded, lowest values are selected regardless of water chemistry and all values are divided by 10	Pessimistic in table A.2.5.2 (Surface diffusion increase is discarded, lowest values are selected regardless of water chemistry and all values are divided by 10	Pessimistic in table A.2.5.2 (Surface diffusion increase is discarded, lowest values are selected regardless of water chemistry and all values are divided by 10

Table A.2.5.2: *Suggested rock diffusivity values. Reasonable estimate correspond to values given by table 2 in Ohlsson and Neretnieks (1997), pessimistic values are the minimum values regardless of water chemistry divided by a factor of 10.*

Element	$D_e \cdot 10^{13}$ [m^2/s]		
	Saline	Fresh	Pessimistic
C/HCO_3	0.50	0.05	0.005
Na/Na (I)	0.54	5	0.05
Cl/Cl	0.83	0.08	0.008
Co/Co (II)	0.29	0.29	0.029
Ni/Ni (II)	0.28	0.28	0.028
Se/Se (IV, VI)	0.4	0.4	0.04
Br/Br	0.83	0.08	0.008
Kr (Inert gas)	0.4	0.4	0.04
Sr/Sr (II)	0.33	3	0.03
Zr/Zr (IV)	0.4	0.4	0.04
Nb/Nb (V)	0.4	0.4	0.04
Tc/TcO_4	0.4	0.04	0.004
Tc/Tc (IV)	0.4	0.4	0.04
Pd/Pd (II)	0.4	0.4	0.04
Ag/Ag (I)	0.71	0.71	0.071
Cd/Cd (II)	0.30	0.30	0.030
Sn/Sn (IV)	0.4	0.4	0.04
I/I	0.83	0.08	0.008
Cs/Cs (I)	0.88	9	0.09
Sm/Sm (III)	0.4	0.4	0.04
Eu/Eu (III)	0.4	0.4	0.04
Ho/Ho (III)	0.4	0.4	0.04
Ra/Ra (II)	0.37	0.37	0.037
Ac/Ac (III)	0.4	0.4	0.04
Th/Th (IV)	0.063	0.063	0.0063
Pa/Pa (IV, V)	0.4	0.4	0.04
U/U (IV)	0.4	0.4	0.04
Np/Np (IV)	0.4	0.4	0.04
Pu/Pu (III, IV)	0.4	0.4	0.04
Am/Am (III)	0.4	0.4	0.04
Cm/Cm (III)	0.4	0.4	0.04

A:2.6 Geosphere sorption

Table A.2.6.1: *Suggested quantification of uncertainties in rock K_d values*

Case	Aberg	Beberg	Ceberg
Reasonable estimate	Reasonable estimate reducing saline values in Table A.2.6.2., taken from Carbol and Engkvist (1997). Use Tc(IV), U(IV) and Np(IV).	Reasonable estimate reducing non-saline values in Table A.2.6.2. taken from Carbol and Engkvist (1997). Use Tc(IV), U(IV) and Np(IV).	Reasonable estimate reducing non-saline values in Table A.2.6.2. taken from Carbol and Engkvist (1997). Use Tc(IV), U(IV) and Np(IV).
Pessimistic	Lowest value in range for saline in Table A.2.6.2.	Lowest value in range for saline in Table A.2.6.2.	Lowest value in range for fresh in Table A.2.6.2.

Table A.2.6.2: *Rock K_d-values (taken from table 12-1 of Carbol and Engkvist, 1997)*

Element	Chemical form / redox state	Saline		Non saline	
		K_d [m^3/kg]	Uncertainty interval	K_d [m^3/kg]	Uncertainty interval
C	HCO3$^-$	0.001	(0.0005-0.002)	0.001	(0.0005-0.002)
Cl	Cl$^-$	0	-	0	-
Co	Co (II)	0.02	(0.01-0.1)	0.1	(0.05-0.5)
Ni	Ni (II)	0.02	(0.01-0.1)	0.1	(0.05-0.5)
Se	Se (-II, IV, VI)	0.001	(0.0005-0.005)	0.001	(0.0005-0.005)
Kr	inert gas	0	-	0	-
Sr	Sr (II)	0.0002	(0.0001-0.001)	0.01	(0.005-0.05)
Zr	Zr (II)	1	(0.5-3)	1	(0.5-3)
Nb	Nb (V)	1	(0.5-3)	1	(0.5-3)
Tc	Tc (IV)	1	(0.3-3)	1	(0.3-3)
Tc	Tc (VII)[*]	0		0	
Pd	Pd (II)	0.01	(0.001-0.05)	0.1	(0.01-0.5)
Ag	Ag (I)	0.05	(0.01-0.1)	0.5	(0.1-1)
Cd	Cd (II)	0.02	(0.01-0.1)	0.1	(0.05-0.5)
Sn	Sn (IV)	0.001	(0-0.01)	0.001	(0-0.01)
I	I$^-$	0	-	0	-
Cs	Cs (I)	0.05	(0.01-0.1)	0.5	(0.1-1)
Sm	Sm (III)	2	(1-5)	2	(1-5)
Eu	Eu (III)	2	(1-5)	2	(1-5)
Ho	Ho (III)	2	(1-5)	2	(1-5)
Ra	Ra (II)	0.02	(0.01-0.1)	0.1	(0.05-0.5)
Ac	Ac (III)	3	(1-5)	3	(1-5)
Th	Th (IV)	5	(1-10)	5	(1-10)
Pa	Pa (IV, V)	1	(0.5-5)	1	(0.5-5)
U	U (IV)	5	(1-10)	5	(1-10)
U	U (VI)*	0.005	(0.001-0.01)	0.01	(0.005-0.02)
Np	Np (IV)	5	(1-10)	5	(1-10)
Np	Np (V)*	0.005	(0.001-0.01)	0.01	(0.005-0.05)
Pu	Pu (III, IV)	5	(1-10)	5	(1-10)
Am	Am (III)	3	(1-5)	3	(1-5)
Cm	Cm (III)	3	(1-5)	3	(1-5)

[*] Represents value for oxidising conditions. Not relevant here.

A:3 Hydrogeology parameters

The following parameters are not directly used in the assessment model chain. The information given here is for reference only.

Table A.3.1 *Suggested quantification of uncertainties in structure models*

Case	Aberg	Beberg	Ceberg
Reasonable estimate	Rhén *et al.* (1997)	Andersson *et al. (*1991).	Hermanson *et al.* (1997).
Pessimistic	Not applicable.	Not applicable.	Not applicable.
Variants	No variant	Additional structures as suggested by Saksa and Nummela (1998).	Additional structures as suggested by Saksa and Nummela (1998).

Table A.3.2 *Suggested handling of repository layout*

Case	Aberg	Beberg	Ceberg
Fixed	As suggested by Munier *et al.* (1997), fig 6-14 and 6-15.	As suggested by Munier *et al.* (1997).	As suggested by Munier *et al.* (1997).

Table A.3.3 *Suggested quantification of uncertainties in hydrogeological models. Table A.3.6 describes which variants were actually analysed within SR 97.*

Case	Aberg	Beberg	Ceberg
Reasonable estimate	Base case as displayed in table A.3.4	Base case as displayed in table A.3.4	Base case as displayed in table A.3.4
Variants (for final selection see table A.3.6)	Discuss or evaluate variants as suggested by Walker *et al. (1997).* (see table A.3.4). In addition uncertainty in boundary conditions to site scale models (see discussion in 6.4) Consider DFN and Channel Network models.	Discuss or evaluate variants as suggested by Walker *et al* (see table A.3.4). New structures suggested by Saksa and Nummela (1998) In addition uncertainty in boundary conditions to site scale models (see discussion in 6.4) Consider DFN and Channel Network models.	Discuss or evaluate variants as suggested by Walker *et al* (see table A.3.4). New structures suggested by Saksa and Nummela (1998) In addition uncertainty in boundary conditions to site scale models (see discussion in 6.4) Consider DFN and Channel Network models.

Table A.3.4a: *Variants in regional scale hydrogeological models as suggested by Walker et al., 1997.*

Variant description	**Aberg - Table 2-10 in Walker *et al.* (1997)**	**Beberg – Table 3-7 in Walker *et al.* (1997)**	**Ceberg - Table 4-6 in Walker *et al.* (1997)**
Rock domain			
Base case	Scaled from on-site packer test data. Depth zones	Scaled from on-site packer test data. Depth zones	Scaled from on-site packer test data. Depth zones
Correlation with rock type	Yes	not suggested	not suggested
Anisotropy	In direction of maximum horizontal rock stress.	In direction of maximum horizontal rock stress	In direction of maximum horizontal rock stress
Conductor domain			
Base case	Regional lineaments of Rhén *et al*, 1997. Depth zones as for base case rock	Mapped lineaments. Hydraulic conductivity inferred from packer tests. No depth zones	Mapped lineaments. Hydraulic conductivity inferred from packer tests. Depth zones.
Alternative depth zones	No depth zones	Depth zones	not suggested
Alternative lineaments	not suggested	Hypothetical sub-horizontal fracture.	Alternative interpretation based on Askling (1997)

Table A.3.4b: *Variants in site scale hydrogeological models as suggested by Walker et al, 1997.*

Description	**Aberg - Table 2-10 in Walker *et al.* (1997)**	**Beberg -Table 3-7 in Walker *et al.* (1997)**	**Ceberg – Table 4-6 in Walker *et al.* (1997)**
Rock domain			
Base case	Upscaled from packer tests assigned to 5 different regions/rock types	Upscaled from packer test, with depth zones.	From packer test, with depth zones
Anisotropy	In direction of maximum horizontal stress	In direction of maximum horizontal rock stress.	In direction of maximum horizontal rock stress.
Conductor domain			
Base case	Fracture zones with properties inferred from interference tests and spinner tests	Fracture zones as in SKB91 no depth zones. Inferred from packer tests	Fracture zones of Hermanson *et al*. (1997), properties and depth zones from packer test data. Uniform for all zones.
Depth zones	not suggested	Depth zones same as for rock domain.	not suggested.
Alternative fracture zones	In accordance with alternative in Rhén *et al* 1997	Hypothetical sub-horizontal fracture zone	Three variants with additional zones.

Table A.3.5 *Suggested quantification of uncertainties in regional models for boundary conditions in the site scale modelling. Table A.3.6 defines which cases were actually analysed in SR 97.*

Case	Aberg	Beberg	Ceberg
Reasonable estimate	Use base case, transfer B.C. as specified head. Select hydraulic conductivity case consistent with site scale selection. Measure potential flux inconsistency between regional and site scale models.	Use base case, transfer B.C. as specified head. Select hydraulic conductivity case consistent with site scale selection. Measure potential flux inconsistency between regional and site scale models.	Use base case, transfer B.C. as specified head. Select hydraulic conductivity case consistent with site scale selection. Measure potential flux inconsistency between regional and site scale models.
Variants	Explore different variants of BC in order to explore impact of transient - density stratification	Discuss impact of transient density stratification	No need for further variants.
For development beyond SR 97	Consider scheme for nested modelling suggested by Follin (1999).	Consider scheme for nested modelling suggested by Follin (1999).	Consider scheme for nested modelling suggested by Follin (1999).

Table A.3.6 *Analysed quantification of uncertainties in hydrogeological models*

Case	Aberg	Beberg	Ceberg
Reasonable estimate	Aberg base case as defined by *Walker and Gylling (1998)* .	Beberg base case as defined by *Gylling et al. (1999a)* .	Ceberg base case as defined by *Walker and Gylling (1999)* .
Variants	1. Boundary conditions 2. Upscaling of LogK 3. Anisotropic Covariance of log K 4. Conditional Simulation of log K 5. Deterministic Simulation DFN-model (Dershowitz *et al*, 1998), Channel Network model (Gylling *et al.*, 1999b), Saline model Svensson 1997b. The latter for qualitative assessment.	1. Environmental head B.C. 2. Additional fracture zones 3. Alternative interpretation of depth dependence and environmental head B.C. 4. Deterministic	1. Increased Fracture Zone contrast 2. Alternative fracture zones 3. Increased variance 4. Deterministic Simulation

A:4 Flow related migration parameters

A:4.1 Suggested handling of spatial variability

Table A.4.1.1: *Suggested handling of spatial variability*

Case	Description
Reasonable estimate	Use ensemble statistics to cover spatial variability. Select median for single value illustration. Do not take credit for emplacement strategy
Pessimistic	Combine the pessimistic near-field, far-field and biosphere parameter values (i.e. assume full correlation between all unfavourable conditions). Do not take credit for emplacement strategy.
Variants	Consider different variants, but still use ensemble statistics to cover spatial variability. As a "what-if" case explore effect of excluding deposition holes (and connected migration paths if applicable) if darcy velocity in this scale exceeds 10^{-1} m/yr, 10^{-2} m/yr or 10^{-3} m/yr.

A:4.2 Flow related migration parameters - near-field

Table A.4.2.1 *Values of W_i and L_i to be used in COMP23 (for definitions see Moreno and Gylling, 1998).*

Path	W_i (m)	L_i (m)
Q1	5	2.8
Q2	1	2.8
Q3	2.5	7.0
Q4	2.5	5.0

Table A.4.2.2 *Quantification of uncertainties in near-field flow Darcy velocity q_0 (m/yr)*

Case	Aberg	Beberg	Ceberg
Reasonable estimate	$2 \cdot 10^{-3}$	$1 \cdot 10^{-3}$	$4 \cdot 10^{-5}$
Pessimistic	10^{-1}	$2 \cdot 10^{-2}$	$2 \cdot 10^{-4}$
Probabilistic	Explore range of Aberg base case (*Walker and Gylling, 1998*)	Explore range of Beberg base case (*Gylling et al., 1999a*)	Explore range of Ceberg base case (*Walker and Gylling, 1999*)

Table A.4.2.3: *Non site specific parameters for input to COMP23*

Parameter	*Reasonable estimate*	*Pessimistic*
Darcy velocities		
q_1	q_0	$5q_0$
q_2	$10q_0$	$100q_0$
q_3	$100q_0$	$1000q_0$
q_4	$100q_0$	$10000q_0$
Porosity		
ε_1	10^{-4}	10^{-3}
ε_2	$3 \cdot 10^{-4}$	10^{-3}
ε_3	10^{-3}	10^{-3}
ε_4	10^{-3}	10^{-3}
The "f_i" parameter in COMP23		
f_1	1	7
f_2	2	13
f_3	25	80
f_4	21	220

A:4.3 Flow related migration parameters - far-field

Table A.4.3.1 *Suggested parameters to FARF31. It should be note that transit time and a_w are correlated and cannot be changed without considering change in the other parameter*

Case	**Aberg**	**Beberg**	**Ceberg**
"Transit time"	yrs	yrs	yrs
Reasonable estimate single	10	60	2000
Pessimistic	0.8	3.3	400
Probabilistic	Base case table 7.3.2	Base case table 7.3.2	Base case table 7.3.2
a_w	(m^{-1})	(m^{-1})	(m^{-1})
Reasonable estimate	10^4	10^4	10^3
Pessimistic	10^3	10^3	10^3
Pe			
Reasonable estimate	10	10	10
Pessimistic	2	2	2
Max penetration	m	m	m
Reasonable estimate	2.0	2.0	20
Pessimistic	0.2	0.2	2.

A:5 Biosphere

Table A.5.1: *Suggested quantification of uncertainties in biosphere module*

Case	**Aberg**	**Beberg**	**Ceberg**
Module			
Reasonable estimate single	Inner bay of Aberg (but compare with well and peat)	Peat (but compare with well)	Peat (but compare with peat)
Pessimistic	Apply the well, peat and soil module select the MODULE resulting in the highest dose.	Apply the well, peat and soil module select the MODULE resulting in the highest dose.	Apply the well, peat and soil module select the MODULE resulting in the highest dose
Probabilistic	Select the module consistent with discharge in Aberg flow case *Walker and Gylling (1998)* selected for probabilistic assessment.	Select the module consistent with discharge in Beberg flow case *Gylling et al. (1999a)* selected for probabilistic assessment.	Select the module consistent with discharge in Ceberg flow case *Walker and Gylling (1999)* selected for probabilistic assessment.
EDF for selected modules			
Reasonable estimate	Median values	Median values	Median values
Pessimistic	Maximum values	Maximum values	Maximum values

***Table A.5.2**. EDF-factors used in the reasonable cases.*

Nuclide	**Reasonable EDF-factors (Sv/Bq)**						
	Aberg			**Beberg**		**Ceberg**	
	Peat area	**Well 300l/h**	**Inner bay**	**Peat area**	**Well 300l/h**	**Peat area**	**Well 300l/h**
Ag-108m	$1.9\cdot10^{-11}$	$1.3\cdot10^{-12}$	$1.1\cdot10^{-15}$	$1.9\cdot10^{-11}$	$1.3\cdot10^{-12}$	$1.8\cdot10^{-11}$	$1.3\cdot10^{-12}$
Am-241	$2.0\cdot10^{-10}$	$6.8\cdot10^{-11}$	$1.6\cdot10^{-14}$	$2.0\cdot10^{-10}$	$6.8\cdot10^{-11}$	$2.0\cdot10^{-10}$	$6.7\cdot10^{-11}$
Am-243	$1.9\cdot10^{-9}$	$1.3\cdot10^{-10}$	$1.6\cdot10^{-14}$	$1.8\cdot10^{-9}$	$1.3\cdot10^{-10}$	$1.7\cdot10^{-9}$	$1.3\cdot10^{-10}$
C-14	$1.1\cdot10^{-14}$	$2.4\cdot10^{-13}$	$1.7\cdot10^{-15}$	$6.5\cdot10^{-15}$	$2.4\cdot10^{-13}$	$4.6\cdot10^{-15}$	$2.4\cdot10^{-13}$
Cl-36	$3.6\cdot10^{-11}$	$7.3\cdot10^{-13}$	$1.6\cdot10^{-16}$	$2.2\cdot10^{-11}$	$7.2\cdot10^{-13}$	$1.5\cdot10^{-11}$	$6.3\cdot10^{-13}$
Cm-245	$1.2\cdot10^{-9}$	$1.6\cdot10^{-10}$	$1.6\cdot10^{-14}$	$9.8\cdot10^{-10}$	$1.6\cdot10^{-10}$	$8.1\cdot10^{-10}$	$1.6\cdot10^{-10}$
Cs-135	$4.4\cdot10^{-12}$	$1.9\cdot10^{-12}$	$7.8\cdot10^{-16}$	$2.7\cdot10^{-12}$	$1.9\cdot10^{-12}$	$1.8\cdot10^{-12}$	$1.7\cdot10^{-12}$
Cs-137	$4.0\cdot10^{-12}$	$5.6\cdot10^{-12}$	$4.8\cdot10^{-15}$	$3.5\cdot10^{-12}$	$5.6\cdot10^{-12}$	$3.1\cdot10^{-12}$	$5.6\cdot10^{-12}$
Ho-166m	$2.3\cdot10^{-12}$	$2.0\cdot10^{-12}$	$1.3\cdot10^{-16}$	$1.9\cdot10^{-12}$	$2.0\cdot10^{-12}$	$1.6\cdot10^{-12}$	$2.0\cdot10^{-12}$
I-129	$5.0\cdot10^{-11}$	$9.2\cdot10^{-11}$	$1.8\cdot10^{-14}$	$3.0\cdot10^{-11}$	$9.1\cdot10^{-11}$	$2.1\cdot10^{-11}$	$7.7\cdot10^{-11}$
Nb-94	$3.0\cdot10^{-12}$	$3.4\cdot10^{-12}$	$2.1\cdot10^{-16}$	$2.0\cdot10^{-12}$	$3.3\cdot10^{-12}$	$1.5\cdot10^{-12}$	$2.8\cdot10^{-12}$
Ni-59	$4.5\cdot10^{-13}$	$5.9\cdot10^{-14}$	$2.2\cdot10^{-17}$	$2.7\cdot10^{-13}$	$5.9\cdot10^{-14}$	$1.9\cdot10^{-13}$	$5.1\cdot10^{-14}$
Ni-63	$1.8\cdot10^{-13}$	$6.2\cdot10^{-14}$	$5.2\cdot10^{-17}$	$1.6\cdot10^{-13}$	$6.3\cdot10^{-14}$	$1.4\cdot10^{-13}$	$6.1\cdot10^{-14}$
Np-237	$1.8\cdot10^{-10}$	$4.7\cdot10^{-11}$	$2.0\cdot10^{-15}$	$1.1\cdot10^{-10}$	$4.7\cdot10^{-11}$	$7.5\cdot10^{-11}$	$4.3\cdot10^{-11}$
Pa-231	$4.7\cdot10^{-9}$	$6.8\cdot10^{-10}$	$1.3\cdot10^{-14}$	$3.5\cdot10^{-9}$	$6.8\cdot10^{-10}$	$2.7\cdot10^{-9}$	$6.7\cdot10^{-10}$
Pd-107	$1.0\cdot10^{-13}$	$2.3\cdot10^{-14}$	$1.2\cdot10^{-18}$	$6.4\cdot10^{-14}$	$2.3\cdot10^{-14}$	$4.4\cdot10^{-14}$	$2.0\cdot10^{-14}$
Pu-239	$6.2\cdot10^{-10}$	$2.2\cdot10^{-10}$	$6.4\cdot10^{-15}$	$4.1\cdot10^{-10}$	$2.3\cdot10^{-10}$	$3.0\cdot10^{-10}$	$2.3\cdot10^{-10}$
Pu-240	$5.2\cdot10^{-10}$	$1.8\cdot10^{-10}$	$6.3\cdot10^{-15}$	$3.6\cdot10^{-10}$	$1.9\cdot10^{-10}$	$2.7\cdot10^{-10}$	$1.9\cdot10^{-10}$
Pu-242	$6.3\cdot10^{-10}$	$2.3\cdot10^{-10}$	$6.1\cdot10^{-15}$	$4.1\cdot10^{-10}$	$2.4\cdot10^{-10}$	$3.0\cdot10^{-10}$	$2.3\cdot10^{-10}$
Ra-226	$1.7\cdot10^{-9}$	$1.2\cdot10^{-10}$	$1.6\cdot10^{-14}$	$1.2\cdot10^{-9}$	$1.1\cdot10^{-10}$	$9.4\cdot10^{-10}$	$1.1\cdot10^{-10}$
Se-79	$2.7\cdot10^{-9}$	$2.7\cdot10^{-12}$	$1.4\cdot10^{-14}$	$1.7\cdot10^{-9}$	$2.7\cdot10^{-12}$	$1.2\cdot10^{-9}$	$2.1\cdot10^{-12}$
Sm-151	$6.4\cdot10^{-15}$	$3.2\cdot10^{-14}$	$5.9\cdot10^{-18}$	$6.0\cdot10^{-15}$	$3.2\cdot10^{-14}$	$5.7\cdot10^{-15}$	$3.2\cdot10^{-14}$
Sn-126	$1.4\cdot10^{-10}$	$3.9\cdot10^{-12}$	$9.9\cdot10^{-16}$	$8.6\cdot10^{-11}$	$3.9\cdot10^{-12}$	$6.1\cdot10^{-11}$	$3.1\cdot10^{-12}$
Sr-90	$2.1\cdot10^{-11}$	$1.3\cdot10^{-11}$	$1.3\cdot10^{-15}$	$1.8\cdot10^{-11}$	$1.3\cdot10^{-11}$	$1.6\cdot10^{-11}$	$1.2\cdot10^{-11}$
Tc-99	$7.0\cdot10^{-13}$	$5.5\cdot10^{-13}$	$1.7\cdot10^{-17}$	$4.2\cdot10^{-13}$	$5.5\cdot10^{-13}$	$2.9\cdot10^{-13}$	$4.7\cdot10^{-13}$
Th-229	$7.5\cdot10^{-9}$	$4.2\cdot10^{-10}$	$1.3\cdot10^{-14}$	$7.0\cdot10^{-9}$	$4.1\cdot10^{-10}$	$6.5\cdot10^{-9}$	$4.1\cdot10^{-10}$
Th-230	$4.4\cdot10^{-9}$	$2.1\cdot10^{-10}$	$5.4\cdot10^{-15}$	$4.0\cdot10^{-9}$	$2.1\cdot10^{-10}$	$3.7\cdot10^{-9}$	$2.0\cdot10^{-10}$
U-233	$1.0\cdot10^{-11}$	$1.9\cdot10^{-11}$	$2.6\cdot10^{-15}$	$6.1\cdot10^{-12}$	$1.9\cdot10^{-11}$	$4.3\cdot10^{-12}$	$1.7\cdot10^{-11}$
U-234	$9.8\cdot10^{-12}$	$1.8\cdot10^{-11}$	$2.5\cdot10^{-15}$	$5.9\cdot10^{-12}$	$1.7\cdot10^{-11}$	$4.1\cdot10^{-12}$	$1.7\cdot10^{-11}$
U-235	$8.9\cdot10^{-12}$	$1.7\cdot10^{-11}$	$2.4\cdot10^{-15}$	$5.4\cdot10^{-12}$	$1.7\cdot10^{-11}$	$3.7\cdot10^{-12}$	$1.6\cdot10^{-11}$
U-238	$8.3\cdot10^{-12}$	$1.6\cdot10^{-11}$	$2.3\cdot10^{-15}$	$5.1\cdot10^{-12}$	$1.6\cdot10^{-11}$	$3.5\cdot10^{-12}$	$1.6\cdot10^{-11}$
Zr-93	$6.1\cdot10^{-13}$	$3.7\cdot10^{-13}$	$9.0\cdot10^{-17}$	$4.4\cdot10^{-13}$	$3.6\cdot10^{-13}$	$3.3\cdot10^{-13}$	$3.6\cdot10^{-13}$

A.5.3. *Pessimistic EDF-factors used in the calculation. In all cases apart from C-14, the EDFs are based on "pessimistic peat". The C-14 EDF is based on the well with the lowest specific capacity at the respective sites.*

Nuclide	**Pessimistic EDF-factors (Sv/Bq)**		
	Aberg	**Beberg**	**Ceberg**
Ag-108m	$2.3\cdot10^{-10}$	$2.3\cdot10^{-10}$	$2.2\cdot10^{-10}$
Am-241	$2.6\cdot10^{-9}$	$2.6\cdot10^{-9}$	$2.6\cdot10^{-9}$
Am-243	$2.7\cdot10^{-8}$	$2.5\cdot10^{-8}$	$2.3\cdot10^{-8}$
C-14	$5.4\cdot10^{-13}$	$2.6\cdot10^{-13}$	$2.6\cdot10^{-13}$
Cl-36	$3.3\cdot10^{-10}$	$2.0\cdot10^{-10}$	$1.4\cdot10^{-10}$
Cm-245	$1.4\cdot10^{-8}$	$1.2\cdot10^{-8}$	$9.4\cdot10^{-9}$
Cs-135	$3.7\cdot10^{-11}$	$2.2\cdot10^{-11}$	$1.5\cdot10^{-11}$
Cs-137	$3.6\cdot10^{-11}$	$2.9\cdot10^{-11}$	$2.6\cdot10^{-11}$
Ho-166m	$2.3\cdot10^{-11}$	$2.0\cdot10^{-11}$	$1.8\cdot10^{-11}$
I-129	$8.2\cdot10^{-10}$	$4.9\cdot10^{-10}$	$3.1\cdot10^{-10}$
Nb-94	$3.3\cdot10^{-11}$	$2.4\cdot10^{-11}$	$1.9\cdot10^{-11}$
Ni-59	$4.1\cdot10^{-12}$	$2.5\cdot10^{-12}$	$1.7\cdot10^{-12}$
Ni-63	$2.0\cdot10^{-12}$	$1.6\cdot10^{-12}$	$1.4\cdot10^{-12}$
Np-237	$1.7\cdot10^{-9}$	$1.0\cdot10^{-9}$	$7.0\cdot10^{-10}$
Pa-231	$5.2\cdot10^{-8}$	$4.3\cdot10^{-8}$	$3.4\cdot10^{-8}$
Pd-107	$1.1\cdot10^{-12}$	$7.1\cdot10^{-13}$	$5.0\cdot10^{-13}$
Pu-239	$7.7\cdot10^{-9}$	$6.4\cdot10^{-9}$	$5.0\cdot10^{-9}$
Pu-240	$6.4\cdot10^{-9}$	$4.9\cdot10^{-9}$	$4.1\cdot10^{-9}$
Pu-242	$8.3\cdot10^{-9}$	$6.8\cdot10^{-9}$	$5.0\cdot10^{-9}$
Ra-226	$1.9\cdot10^{-8}$	$1.6\cdot10^{-8}$	$1.2\cdot10^{-8}$
Se-79	$2.6\cdot10^{-8}$	$1.7\cdot10^{-8}$	$1.2\cdot10^{-8}$
Sm-151	$8.4\cdot10^{-14}$	$8.1\cdot10^{-14}$	$7.7\cdot10^{-14}$
Sn-126	$1.4\cdot10^{-9}$	$9.1\cdot10^{-10}$	$6.3\cdot10^{-10}$
Sr-90	$2.2\cdot10^{-10}$	$1.8\cdot10^{-10}$	$1.6\cdot10^{-10}$
Tc-99	$1.8\cdot10^{-11}$	$1.1\cdot10^{-11}$	$7.4\cdot10^{-12}$
Th-229	$9.9\cdot10^{-8}$	$8.6\cdot10^{-8}$	$8.2\cdot10^{-8}$
Th-230	$5.7\cdot10^{-8}$	$5.0\cdot10^{-8}$	$4.5\cdot10^{-8}$
U-233	$1.4\cdot10^{-10}$	$8.7\cdot10^{-11}$	$6.0\cdot10^{-11}$
U-234	$1.4\cdot10^{-10}$	$8.4\cdot10^{-11}$	$5.9\cdot10^{-11}$
U-235	$1.3\cdot10^{-10}$	$7.6\cdot10^{-11}$	$5.3\cdot10^{-11}$
U-238	$1.2\cdot10^{-10}$	$7.2\cdot10^{-11}$	$5.0\cdot10^{-11}$
Zr-93	$4.8\cdot10^{-12}$	$3.5\cdot10^{-12}$	$2.8\cdot10^{-12}$

Table A.5.4 *Pessimistic EDF-factors used in the probabilistic calculations.*

Nuclide	Pessimistic EDF-factor (Sv/Bq)					
	Aberg		Beberg		Ceberg	
	Peat area	Well 300l/h	Peat area	Well 300l/h	Peat area	Well 300l/h
Ni-59	$4.1\cdot10^{-12}$	$2.0\cdot10^{-13}$	$2.5\cdot10^{-12}$	$2.0\cdot10^{-13}$	$1.7\cdot10^{-12}$	$1.6\cdot10^{-13}$
Nb-94	$3.3\cdot10^{-11}$	$8.3\cdot10^{-12}$	$2.4\cdot10^{-11}$	$8.3\cdot10^{-12}$	$1.9\cdot10^{-11}$	$7.3\cdot10^{-12}$
Sn-126	$1.4\cdot10^{-9}$	$1.2\cdot10^{-11}$	$9.1\cdot10^{-10}$	$1.2\cdot10^{-11}$	$6.3\cdot10^{-10}$	$8.4\cdot10^{-12}$
I-129	$4.7\cdot10^{-10}$	$3.7\cdot10^{-10}$	$2.8\cdot10^{-10}$	$3.6\cdot10^{-10}$	$2.0\cdot10^{-10}$	$2.7\cdot10^{-10}$
Ra-226	$1.9\cdot10^{-8}$	$2.2\cdot10^{-10}$	$1.6\cdot10^{-8}$	$2.1\cdot10^{-10}$	$1.2\cdot10^{-8}$	$1.9\cdot10^{-10}$
Th-230	$5.7\cdot10^{-8}$	$5.3\cdot10^{-10}$	$5.0\cdot10^{-8}$	$5.2\cdot10^{-10}$	$4.5\cdot10^{-8}$	$5.1\cdot10^{-10}$
U-234	$1.4\cdot10^{-10}$	$2.9\cdot10^{-11}$	$8.4\cdot10^{-11}$	$2.9\cdot10^{-11}$	$5.9\cdot10^{-11}$	$2.7\cdot10^{-11}$
U-238	$1.2\cdot10^{-10}$	$2.6\cdot10^{-11}$	$7.2\cdot10^{-11}$	$2.5\cdot10^{-11}$	$5.0\cdot10^{-11}$	$2.4\cdot10^{-11}$
Pu-239	$7.7\cdot10^{-9}$	$6.0\cdot10^{-10}$	$6.4\cdot10^{-9}$	$6.0\cdot10^{-10}$	$5.0\cdot10^{-9}$	$6.0\cdot10^{-10}$

Table A.5.5 *Reasonable EDF-factors for "Open Coast" used in the glacial melting scenario for Aberg.*

Nuclide	Reasonable EDF-factor (Sv/Bq) Open Coast Aberg
Ag-108m	$4.3\cdot10^{-18}$
Am-241	$2.0\cdot10^{-16}$
Am-243	$2.0\cdot10^{-16}$
C-14	$6.7\cdot10^{-18}$
Cl-36	$5.7\cdot10^{-19}$
Cm-245	$2.1\cdot10^{-16}$
Cs-135	$2.9\cdot10^{-18}$
Cs-137	$1.8\cdot10^{-17}$
Ho-166m	$1.9\cdot10^{-18}$
I-129	$1.1\cdot10^{-16}$
Nb-94	$1.5\cdot10^{-18}$
Ni-59	$9.0\cdot10^{-20}$
Ni-63	$2.1\cdot10^{-19}$
Np-237	$7.6\cdot10^{-18}$
Pa-231	$4.8\cdot10^{-17}$
Pd-107	$2.6\cdot10^{-20}$
Pu-239	$5.5\cdot10^{-17}$
Pu-240	$5.5\cdot10^{-17}$
Pu-242	$5.3\cdot10^{-17}$
Ra-226	$7.0\cdot10^{-17}$
Se-79	$5.3\cdot10^{-17}$
Sm-151	$9.1\cdot10^{-20}$
Sn-126	$3.8\cdot10^{-18}$
Sr-90	$5.0\cdot10^{-18}$
Tc-99	$6.1\cdot10^{-19}$
Th-229	$4.0\cdot10^{-16}$
Th-230	$1.7\cdot10^{-16}$
U-233	$1.1\cdot10^{-17}$
U-234	$1.1\cdot10^{-17}$
U-235	$1.0\cdot10^{-17}$
U-238	$9.7\cdot10^{-18}$
Zr-93	$9.8\cdot10^{-19}$

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