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Abstract

This report concerns the selection of flow related transport parameters for the SR 97 safety assessment project. Interrelationships of the parameters controlling migration and matrix diffusion in the far-field and the issue of spatially varying properties along the migration paths are discussed. Available field information on porosity, flow wetted surface and dispersivity from Aberg, Beberg and Ceberg are explored and values and uncertainty ranges to be used in the assessment calculations are suggested. It is shown how to combine results from the hydrogeological modelling of SR 97 with the data estimates in order to produce parameters to the source term and far-field migration codes.

Evaluation of migration and matrix diffusion along varying flow paths demonstrates that the assessment relevant parameter for migration modelling of sorbing elements is the ”F-quotient”. If averaged along a flow path the F-quotient could alternatively be expressed in terms of the quotient between the ”flow wetted surface per volume of rock” times the migration path length and the Darcy velocity ($a_r L/q$), or as the product between water ”transit time” and flow wetted surface per volume of water. In a spatially varying flow field the proper means of defining these average properties are not self evident. However, it can be shown that the sum of the F-quotient in a series of segments, where properties are constant within each segment, can be used as an effective F-quotient for the entire migration path. For non-sorbing species the F-quotient is not sufficient to describe transport. Dispersion, modelled as a Peclet number, is far less important than the F-quotient for sorbing species, at least for Peclet numbers larger than 2.

The site specific transport relevant information available for the SR 97 sites comprise tracer tests, geological characterisation, hydraulic measurements, and modelling. It appears that the most defensible means of estimating the flow wetted surface per volume of rock would be through estimates of conductive fracture frequency. These measures could be estimated from all three sites using hydraulic data, but the resolution of data from Ceberg is quite poor.

Sammanfattning

Denna rapport syftar till att ta fram flödesrelaterade transportparametrar för säkerhetsanalysen SR 97. Rapporten diskuterar relationen mellan de olika parametrar som styr migration och matrisdiffusion när flödet och flödets geometri varierar längs transportvägarna. Tillgängliga fältdata om porositet, flödesvätt yta och dispersivitet från Aberg, Beberg och Ceberg utvärderas och förslag till parametervärden att använda i konsekvensanalysen, tillsammans med osäkerhetskattningar, föreslås. Analysen visar även hur resultat från den hydrogeologiska modelleringen i SR 97 kan kombineras med dessa parametervärden, för att kunna ta fram parametervärden till beräkningskoderna för källterm och fjärrområdestransport.

Analysen av transport och matrisdiffusion längs varierande flödesvägar visar att det är den s.k. "F-kvoten" som har störst inverkan på transporten av sorberande ämnen. Om transportvägens egenskaper är konstanta i rummet kan F-kvoten antingen uttryckas som kvoten mellan "flödesvätta ytan per volym berg" och Darcy-hastigheten multiplicerat med transportsträckan ($a_r L/q$), eller som produkten mellan (den icke-sorberade) "transport tiden" och "flödesvätta ytan per volym vatten". Om flödesfältet varierar längs transportvägen är det däremot inte uppenbart hur meningsfulla medelvärden av dessa storheter ska formuleras. Man kan dock visa att summan av "F-kvoter" för enskilda segment i en serie, där flödet och geometrin är konstant inom varje segment, kan användas som en effektiv F-kvot för hela transportsträckan. För icke-sorberande ämnen räcker det inte att bara känna till F-kvoten, då behövs även kunskap om transporttiden. För sorberande ämnen är vidare dispersion mindre viktig, åtminstone för Peclet-tal större än 2.

För SR 97 finns platsspecifik information om tranportegenskaper i form av resultat av spårförsök, geologisk karakterisering, hydrauliska mätningar och modellering. Det tycks som om den mest försvarbara metoden att skatta den flödesvätta ytan per volym berg är att utnyttja skattningar av den konduktiva sprickfrekvensen. Detta mått kan skattas från hydrauliska mätningar, vilket gör det möjligt att erhålla skattningar från alla tre platser. Upplösningen i värdena från Ceberg är dock dålig, varför de skattade parametervärdena därifrån blir extra osäkra.

Executive summary

This report concerns the selection of flow related transport parameters for the SR 97 safety assessment project. SR 97 evaluates three different hypothetical sites, Aberg, Beberg and Ceberg with data taken from Äspö, Finnsjön and Gideå respectively. The direct radiological consequence analyses are performed by a near-field source term code, a far-field migration code and a biosphere code. The groundwater flow modelling of SR 97 primarily serves as input to these consequence calculations.

The present report has the following specific purposes:

- it discusses the interrelationships of the parameters controlling migration and matrix diffusion in the far-field and the issue of spatially varying properties along the migration paths,

- it explores available field information on porosity, flow wetted surface and dispersivity from Aberg, Beberg and Ceberg and it suggests values and uncertainty ranges to be used in the assessment calculations,

- it discusses how to combine results from the hydrogeological modelling of SR 97 with the data estimates suggested in this report in order to produce parameters to the source term and far-field migration codes.

Important to the estimation of the flow wetted surface is the question whether the full fracture surface is available for matrix diffusion or if only a part of the fracture make up a flow wetted surface. SR 97 would need to apply a rather conservative view on this issue, but research on the migration in a single fracture with varying velocity field is recommended.

Evaluation of migration and matrix diffusion along varying flow paths demonstrates that the assessment relevant parameter for migration modelling of sorbing elements is the "F-quotient", which alternatively could be expressed in terms of the quotient between the flow wetted surface per volume of rock times the migration path length and the Darcy velocity (a_rL/q), or as the product between water "transit time" and flow wetted surface per volume of water (a_wt_w). The "F-quotient" for a migration path made up of many small segments each with different flow and geometry is approximately the sum of the F-quotients for the individual segments ($F_{tot}=\Sigma F_i$). It should be noted that the flow wetted surface area per volume of water, a_w, is inversely proportional to flow porosity, ε_f, (and thus to transit time), whereas the link is far less strong between flow porosity and flow wetted area per volume of rock, a_r. In a heterogeneous medium the average value of a_w is generally not equal to the quotient a_r/ε_f.

It is demonstrated that the sum of the F-quotient in individual segments can be used as an effective F-quotient for the entire migration path. For non-sorbing species the F-quotient is not sufficient to describe transport as then the advective velocity determines migration times, but this is of relatively minor importance in performance assessment.

Further background work may be needed on the issue of dispersion. However, the multiple stream tube approach adopted implies that within each tube the dispersion term only needs to capture the variability of t_{tot} and F_{tot} *within* the tube. The variability *between* tubes is taken care of using multiple tubes. Furthermore, the Peclet number is far less important than the F-quotient for sorbing species, at least for Peclet numbers larger than 2. At Peclet numbers higher than 50 the spreading effect of matrix diffusion and sorption will completely dominate the shape of the release at the outlet. For Peclet numbers higher than 100 dispersion will have no effect on the release from the geosphere.

The site specific transport relevant information available for the SR 97 sites comprises tracer tests, geological characterisation, hydraulic measurements, and modelling. It appears that the most defensible means of estimating the flow wetted surface per volume of rock (a_r) would be through estimates of conductive fracture frequency (CFF) and the related property conductive fracture intensity (P_{32c}). These measures could be estimated from all three sites using hydraulic data, but the resolution of data from Ceberg is quite poor. The table below displays the suggestions for flow related transport parameters for use in SR 97 with best estimate and range. Motives for these suggestions are provided in the report.

Table Suggested flow related transport parameters for use in SR 97 with best estimate and range.

Type of data	*Aberg*	*Beberg*	*Ceberg*
Flow wetted surface - a_r (m^{-1})			
All domains	1.0 (10 - 0.1)	1.0 (10 - 0.1)	0.1 (1. - 0.01)
Flow porosity ε_f			
All domains	10^{-3} (10^{-4} - 10^{-2})	10^{-3} (10^{-4} – 10^{-2})	10^{-3} (10^{-4} - 10^{-2})
Pe-number			
All domains	10 (2-50)	10 (2-50)	10 (2-50)

In addition the following can be noted:

- Only limited data exist within SR 97 for direct estimates of the flow wetted surface. In future development there is reason to explore for other sources of information.
- There is currently no clear experimental support for assigning different values of a_r to different parts of the rock (such as major discontinuities and the rock between these discontinuities). There is probably such a correlation for flow porosity (ε_f), but given the present incapability of properly handling varying flow porosity in assessment codes (see chapter 5) a single value is still suggested for SR 97. More precise parameter estimates would be needed to further substantiate such a conclusion and

proper means of handling it would need to be developed before it could be considered in performance assessment.

- Estimates of F-quotients (or complete input data sets to FARF31) from alternative models appear to be an important complement to the direct estimation of a_r. Such analyses are also planned within SR 97.

SR 97 uses the COMP23 code for the near-field migration and FARF31 for the far field migration analyses. The direct input parameters to FARF31 are the total migration time t_{tot} and the flow wetted surface per volume of water $a_{w,glob}$. As already pointed out these parameters are strongly correlated. This can be handled by selecting $a_{w,glob}=F_{tot}/t_{tot}=\Sigma F_i/t_{tot}$. The groundwater flow modelling of SR 97 primarily serves as input to the assessment calculations. The approach adopts a stochastic continuum model, HYDRASTAR. In addition, discrete fracture network (FracMan/PAWorks) and channel network modelling (CHAN3D) are used in a few cases. It is shown how the output from these codes can be adjusted to suite the needs of the source term and migration codes.

In conclusion, it is clear that site specific estimates of flow related migration parameters could only be made within broad ranges. In order to improve precision in these estimates, and thus potentially decrease uncertainty ranges in future assessments, both theoretical and experimental development is needed. It is strongly recommended that special analyses are initiated, which may resolve some of the issues which now have to be treated with variations and conservative assumptions. The following is suggested:

- develop the theoretical understanding of migration and matrix diffusion,
- study the effect of diffusion into stagnant or low flow zones in a single fracture,
- migration modelling directly in the flow codes,
- exploring for further evidence of matrix diffusion from tracer tests, static diffusion tests, geology and geochemistry.

This may potentially result in a better perspective on the flow wetted surface values actually selected and could also show a way further on how to reduce uncertainties in the estimates in coming performance assessments.

Contents

1 Introduction

This report concerns the selection of flow related transport parameters for the SR 97 safety assessment project. A prime objective of SR 97 is to explore the safety function of a nuclear waste repository for the geological conditions that could occur within potentially possible sites in the Swedish crystalline basement rock. SR 97 evaluates three different hypothetical sites, Aberg, Beberg and Ceberg with data taken from Äspö, Finnsjön and Gideå respectively. In the following, this report will refer to the different sites using the names Aberg, Beberg and Ceberg, but will provide proper references to the data from these sites.

One important part of the SR 97 assessment is to evaluate the radiological consequences of failed canisters as this may lead to release from the spent fuel and subsequent migration to the biosphere. The primary tool used for evaluating this scenario is made up of a series of coupled models, which in turn require input from analyses of the state of the barriers and the rock. A near-field source term code, a far-field migration code and a biosphere code perform the direct radiological consequence analyses. The various sources of information to these codes could in turn build on elaborate modelling combined with data analysis. The input needs to source term and far field migration models can roughly be divided into parameters controlling mobility (solubilities, sorption properties, matrix diffusivity, etc.) and flow related ones concerning groundwater flow and its geometrical distribution in the rock. This report concerns the latter, whereas the derivation of the mobility parameters is handled by other reports within SR 97.

The groundwater flow modelling of SR 97 primarily serves as input to the consequence calculations. The underlying conceptual model of the rock assumed (Walker *et al.*, 1997) 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 (Norman, 1992) embedded in a regional scale model with less geometrical detail and with equivalent, i.e. non-stochastic, hydraulic parameters. In addition, discrete fracture network (Dershowitz *et al.*, 1998) and channel network modelling (Gylling *et al.*, 1998) are used in a few cases as alternative means for deriving input to the consequence models.

The source term code, CHAN3D (Romero *et al.*, 1995), uses the Darcy velocities calculated by groundwater models, but also needs information on porosity and fracture geometry in the near-field environment. The transport code, FARF31 (Norman and Kjellbert, 1992), uses a a streamtube approach where particle "travel times", and discharge locations of a set of one-dimensional streamtubes are obtained from particle tracking in the flow model. In addition, the code needs information on the "flow wetted surface per volume of water" a_w, and the "Peclet"-number. All these parameters, however, are interrelated and it needs to be understood that they cannot be selected independently from each other. The model parameters rather should be seen as mathematical entities to be selected such that the modelling result is meaningful and not as parameters with well defined physical meaning. The "travel time" in particular should not be confused with the "real" migration time of a sorbing or non-sorbing tracer. Previous safety assessments such as TVO-92 (Vieno *et al.,* 1992) or SKI SITE-94 (SKI, 1996) demonstrate that the migration of sorbing species essentially depends on the quotient between the flow wetted surface per volume of rock times the path length and the darcy velocity (a_rL/q), which in turn equals the product of the "travel time" and the flow wetted surface per volume of water. Furthermore, in reality both the flow and the specific surface area vary along the migration path, which raises the question how to properly average these properties into the migration code parameters.

Apart from properly abstracting migration information from the flow codes it is also necessary to obtain field information on the geometry of flow paths. Elert (1997) has already explored different concepts and data for matrix diffusion and flow wetted surface parameters, but not on the specific SR 97 sites.

The present report has the following specific purposes:

- it discusses the interrelationships of the parameters controlling migration and matrix diffusion in the far-field and the issue of spatially varying properties along the migration paths,
- it explores available field information on porosity, flow wetted surface and dispersivity from Aberg, Beberg and Ceberg and it suggests values and uncertainty ranges to be used in the assessment calculations,
- it discusses how to combine results from the hydrogeological modelling of SR 97 with the data estimates suggested in this report in order to produce parameters to the source term and far-field migration codes.

Finally, it needs to be stressed that difficulties in assigning proper values of matrix diffusion and flow wetted surface is not so much a modelling issue as an issue of knowledge and understanding of the fractured rock. The main uncertainties are the same for any of the model concepts considered in SR 97.

2 Migration and matrix diffusion

This section outlines some of the issues that need to be handled in migration modelling. It also discusses how to derive effective parameters if migration properties vary along the migration paths. However, it does not discuss how to estimate these parameters from field data. This will be discussed in the next chapter.

2.1 Introduction

In an overview of retention mechanisms and the flow wetted surface Elert (1997) concluded that:

- At present no single method for determining the flow wetted surface is available that satisfies all requirements concerning giving relevant values, covering relevant distances and being practical to apply. Instead a combination of methods must be used.
- In the safety assessment modelling focus should be put on the quotient between flow wetted surface per volume of rock and water flux, since it has been found to be a more appropriate parameter to describe the efficiency of retardation in the rock than the flow wetted surface.
- The long-term research should address both the detailed flow within the fractures and the effective flow wetted surface along the flow paths. Focus should be put on the transport of sorbing radionuclides, if possible using analogues such as heat transport.

Further details on some of the concepts of flow wetted surface and matrix diffusion are given by Vieno *et al.* (1992), Moreno *et al.* (1997) and by Selroos and Cvetkovic (1996). The present section will focus on some issues of potential importance for the SR 97 study.

2.2 The "flow wetted surface" in a single fracture

Important to the estimation of the flow wetted surface is the question whether the full fracture surface is available for matrix diffusion or if only a part of the fracture make up a flow wetted surface. It appears to be evident that:

- in a heterogeneous fracture, streamlines will be concentrated to a limited part of the fracture surface and in the remainder of the fracture either the two surfaces will be in direct contact or the fracture will contain isolated pools with practically stagnant water (Figure 2.1 a),
- there is no migration in the parts of the fracture with direct rock/rock contacts,

- movement of the diffusion front into the "non-flow" part of the fracture is fast, but will be significantly retarded due to diffusion from the fracture into the surrounding matrix.

The additional flow wetted surface available in the water filled parts "outside" the main flow path will depend upon how efficient the transport into the "non-flow" part is in relation to the matrix diffusion in that part of the fracture. This will in turn depend on the dispersion in the fracture, the diffusion resistance into the "non-flow" part of the fracture (a function of fracture aperture, b, and diffusivity in the fracture, D) and the matrix diffusion in the "non-flow" part of the fracture (a function of K_d, matrix diffusivity, D_m, matrix porosity, ε_m and time). See Figure 2.1.

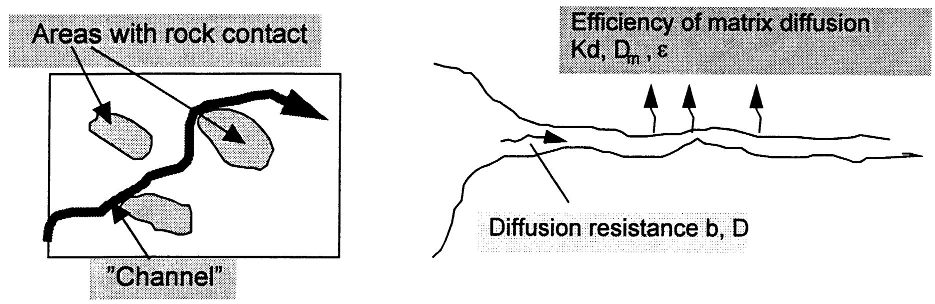

Figure 2.1 :Flow wetted surface in the plane (left) and in a normal cross-section (right) of a heterogeneous fracture

However, there seems to be a lack of quantitative investigations of these effects. A simple transport model for flow in fractures considering diffusion into small aperture regions have been developed by Johns and Roberts (1991). In the TVO-92 study (Vieno *et al.* 1992), the effect of stagnant pools was made considering only the effect of a stagnant water phase. The results indicated that the stagnant pools may have a more significant effect than matrix diffusion for weakly sorbing radionuclides.

It has been suggested that geochemical evidence ("red colouring") may be used for estimating the flow wetted surface locally. Mazurek *et al.* (1996) have made a detailed characterisation of over 80 water conducting fractures at Äspö, but have so far not directly estimated any migration parameters.

At present a pragmatic approach is probably to assume that only a certain percentage (say 10%) of the flowing fracture surface actually contributes to matrix diffusion. Such assumptions were made in TVO-92 for the intact rock and was one of the approaches taken in SKI SITE-94 (SKI, 1996). However, it appears to be possible to improve such an estimate by performing numerical studies in a spatially varying fracture plane using actually measured aperture distributions and realistic source sizes. Such improvements, however, lie outside the scope of SR 97.

2.3 "Effective" flow wetted surface, transit time and flow - in a network of fractures along a single path

The question has been raised whether it is possible to combine a series of fractures, with different sizes and flow into a single value of the flow wetted surface representing the entire flow path. It turns out that this is in fact possible, at least as long as dispersion does not dominate the problem. At least partly these questions have been analysed by Lee *et al.* (1990) and also Selroos and Cvetkovic (1996) who discuss and derive global parameters along a flow path for a general geometry. Below follows a more heuristic derivation of such global properties, made for the special case with a surface sorbing species and a special geometry.

Consider a series of connected plane parallel fractures shown in Figure 2.2, where the network may consist of different branches such that the groundwater flux may differ in different fractures along a flow path. Let fracture *i* have the following "properties":

Q_i = flow rate (L^3T^{-1})

W_i = width (L)

L_i = length (L)

e_i = aperture (L)

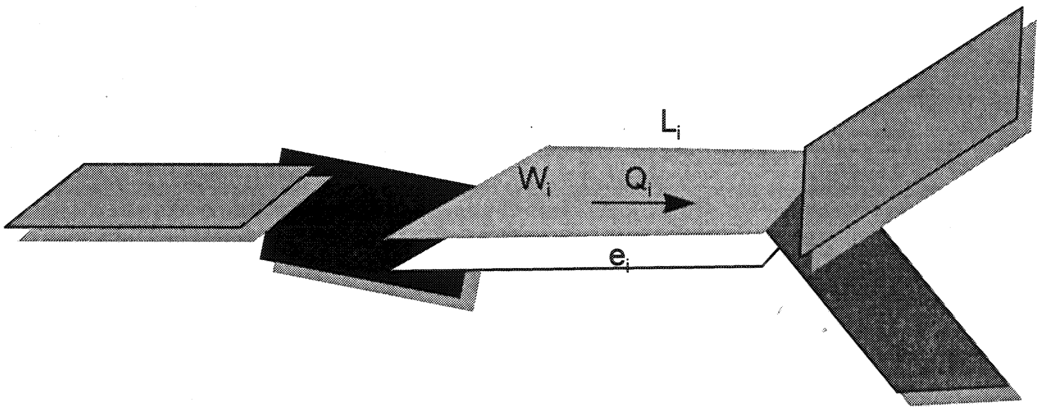

Figure 2.2: A series of connected fractures of different sizes and different fluxes (i.e. a network can consists of branching paths).

For a non-sorbing tracer the travel time through the fracture can be written as:

$$t_i = (W_i\, e_i\, L_i) / Q_i = L_i/v_i \tag{2.1}$$

where v_i is the velocity in the fracture.

For a surface sorbing tracer the travel time through the fracture can be written as:

$$t_{s,i} = L_i / v_{s,i} \tag{2.2}$$

where $v_{s,i}$ = velocity of the front (LT^{-1}). $v_{s,i}$ can be written as:

$$v_{s,i} = Q_i / \{W_i (e_i + 2 K_a)\} \approx Q_i / (2 K_a W_i) \tag{2.3}$$

The approximation in the last step can be made since $e_i << K_a$ even for only slightly sorbing radionuclides. Combining (2.1- 2.3) gives:

$$t_{s,i} = ((e_i+2 K_a)W_i L_i) / Q_i = t_i+2K_aW_iL_i/Q_i \approx 2K_aW_iL_i/Q_i \tag{2.4}$$

We now introduce the F parameter ($T L^{-1}$) which is the quotient between flow wetted area and water flow rate:

$$F_i= 2 W_i L_i / Q_i \tag{2.5}$$

and by inserting (2.5) in (2.4) we obtain:

$$t_{s,i}=t_i+K_aF_i \tag{2.6}$$

By using the relation: $Q_i = v_iW_ie_i$ and defining the flow wetted area per volume of water, $a_{wi}=2/e_i$ the F-quotient can also be expressed as:

$$F_i = t_i a_{wi} \tag{2.7}$$

It needs to be pointed out that equation 2.7 may lead to the misunderstanding that t_i, e_i (or flow porosity) taken separately are important parameters for determining radionuclide migration. Since t_i is proportional to e_i and a_{wi} inversely proportional to e_i equation 2.7 in fact demonstrates that the local value of e_i cancels out. In contrast W_i, L_i and Q_i in equation 2.5 are much more (if not fully) independent of each other, which makes it more justified to try to assess these parameters rather than t_i and a_{wi}.

From any release point the migration path would consist of several interconnected fractures (in series). The total travel time for a non-sorbing tracer in any such pathway consisting of many fractures becomes:

$$t_{tot} =\Sigma t_i \tag{2.8}$$

The total travel time for a sorbing tracer is the sum of the times in the individual fractures, which in turn is a function of the sum of the F-quotients for the individual fractures since:

$$t_{s,tot} = \Sigma t_{s,i} = t_{tot}+K_a \Sigma F_i = t_{tot}+K_a F_{tot} \approx K_aF_{tot} \tag{2.9}$$

i.e., generally, the travel time is a function of the non-sorbing travel time, t_{tot}, and the sum of the F-quotients, but in practice the non-sorbing travel time can be neglected for sorbing tracers, making the F-quotient the only really important number.

Defining $F_{tot} = t_{tot} a_{w,glob}$ we may then derive an expression for $a_{w,glob}$:

$$a_{w,glob} = \Sigma F_i /t_{tot} \tag{2.10}$$

The relations provided above could also be described within the framework of a "porous medium" description. Introducing the darcy velocity $q_i=Q_i/A_i$, and the flow wetted surface per volume of rock $a_{r,i}=2W_i/A_i$, where A_i is an (arbitrary) cross-section area, transfers equation (2.1) into

$$t_i=q_i/\varepsilon_{f,i} \tag{2.11}$$

where $\varepsilon_{f,i}=e_iW_i/A_i$, and equation (2.7) into

$$F_i=a_{r,i}L_i/q_i \tag{2.12}$$

One should note that these two definitions of F_i (2.7 and 2.11) are equivalent, but that in general the average value of $a_{w,glob} \neq a_{r,glob}/\varepsilon_{f,glob}$ as a_{wi} usually is strongly correlated to $\varepsilon_{f,i}$. The proper way of averaging, if sorption properties are to be retained, is to use equations 2.9 and 2.10 and make sure that the F-value is preserved.

The evaluation demonstrates that the concept "flow wetted surface per volume of water", a_w, is strongly correlated to flow porosity. Consequently, an assessment of "groundwater travel times" which is a function of both Darcy velocity and flow porosity, *cannot be made independent* of assessments of the a_w. In contrast $\Sigma(a_{r,i}L_i/q_i)$ can be estimated without explicit knowledge of porosity and aperture.

The derivation in equations 2.1 - 2.12 builds on the assumption of piece wise parallel plate fractures. However, Selroos and Cvetkovic (1996), using a somewhat different notation, demonstrate that in general varying field the summation in equation 2.9 can be replaced by an integral.

2.4 Effect of matrix diffusion

The effect of matrix diffusion also depends on matrix diffusivities, porosities and K_d-values. The matrix properties may vary along the flow tube as well as perpendicular to it. Of particular interest is the issue whether there is a correlation between flow paths of certain flow properties and the available matrix porosity along paths.

Also matrix diffusion depends upon the quotient flow wetted surface and water flow rate (F_i) as can be shown following the derivation of Carslaw and Jaeger (1959) for the analogue problem of heat transport in heat exchangers. The solution, which is a function of the sum of F-quotients, is shown to be strictly valid for the case with no dispersion and an infinite depth of the matrix diffusion.

For the simple case with no dispersion in the fracture and matrix diffusion into an infinite matrix, a simple analytical solution can be derived. For this case, the F-quotient approach can be expanded in order to take into account matrix diffusivity, matrix porosity and the distribution coefficient, obtaining the following (Vieno et al., 1992):

$$C_f(L_i,t) = C_0\mathrm{erfc}(u_i t^{-1/2})$$

$$u_i = a_{r,i}\, L_i\, \mathrm{sqrt}\, [\, D_{m,i}\, (\varepsilon_{m,i} + K_{d,i}\, \rho)] \,/\, q_i$$

$$= F_i \cdot \mathrm{sqrt}\ [\ D_{m,i}\ (\varepsilon_{m,i}\ + K_{d,i}\ \rho)] \tag{2:13}$$

where C_f is the water phase concentration at distance L_i at time t and C_0 is the initial concentration at the source. For significantly sorbing radionuclides the expression can be simplified to:

$$u_{sorb} \approx F_i\ \mathrm{sqrt}\ [\ D_{m,i}\ K_{d,i}\ \rho] \tag{2:14}$$

and for non-sorbing radionuclides as:

$$u_{nonsorb} \approx F_i\ \mathrm{sqrt}\ [\ D_{m,i}\ \varepsilon_{m,i}] \tag{2:15}$$

The u-parameter has the dimension $T^{1/2}$. In a flow path with different segments, the solution depends on the sum of the u values (see also Lee *et al.,* 1990, for an analytical solution for multiple pathways combined with matrix diffusion).

Equations (2:13-2:15) indicate that the sum of the F-quotients (in equations 2:1-2:11) determines the transport as long as $D_{m,i}$ and $K_{d,i}$ are constant. In SR 97 this will also be assumed to be the case, which means that the F-quotient is the key migration parameter. Generally, also $D_{m,i}$ and $K_{d,i}$ vary along the flow path and then proper averaging must preserve the u value rather than the F-value. In general it would not be correct just to use average values of $a_{r,i}$, L_i, q_i, $D_{m,i}$ and $K_{d,i}$.

The extension is less straight-forward for cases with important dispersion in the fracture or a finite penetration depth of the matrix. However, similar terms appear in the analytical solution derived by Tang *et al.* (1981), who address this situation.

2.5 Dispersion

The previous section discussed migration and matrix diffusion along a single migration path. However, in general migration may take place over multiple paths with different migration properties. Multiple paths may occur due to a distributed source which will "discharge" into many paths, by branching of a single path e.g. in fracture intersections or by a combination of these phenomena.

The detailed scale flow modelling practised by SKB considers different concepts such as the stochastic continuum model, the discrete fracture network model and the channel network model. In abstracting such flow model information to the migration modelling, the flow field is divided into multiple single flow tubes obtained e.g. by particle tracking, where each tube represents the track from an individual potential canister position. A one-dimensional advection dispersion model (FARF31, Norman and Kjellbert, 1990) is then applied to each tube.

Analysing multiple single tubes, implies that within each path the dispersion term only needs to capture the variability of t_{tot} and F_{tot} *within* the tube. The variability *between* tubes is taken care of by using multiple tubes.

If the flow field was fully known it would, in principle be possible to calculate t_{tot} and F_{tot} for each path and thereby produce a distribution of t_{tot} and F_{tot} as a function of the release point. However, some averaging of the flow field is almost always necessary in modelling, which means that the distribution of t_{tot} and F_{tot} inside the tube needs to be handled by other means.

The traditional way of handling the variability in flow paths is by modelling small scale multiple paths as an averaged flow field, sometimes described as a set of single "flow tubes", and to describe the variability of the flow field by including a dispersion term, which will cause a spread similar to "fickian" dispersion. It should be noted that the advection-dispersion equation, also including its general three-dimensional formulation which builds on an assumption of a fairly smooth (i.e. averaged) velocity field, is such a model. The magnitude of the dispersion term in the model depends on the resolution of the velocity field. Consequently, the dispersion coefficient is a modelling concept rather than a physical parameter.

Dispersion can be described by the dispersion coefficient D or by the dispersion length α_L related to D by:

$$D = \alpha_L \cdot v \qquad (2.16)$$

where v is the advective velocity. It is also common to introduce a Peclet-number relating the dispersive and the advective fluxes i.e.

$$Pe = Lv/D = Lv/(\alpha_L \cdot v) = L/\alpha_L \qquad (2.17)$$

where L is the migration distance. However, generally neither D, α_L nor Pe are constants. Field and laboratory experiments in fractures and fractured rock evaluated by the advection-dispersion model (i.e. usually assuming a uniform velocity field) often result in a dispersion coefficient (or the dispersion length) which increases with the length of the flow path (see e.g. Gelhar *et al.,* 1992). Experience thus indicates that the dispersion length is proportional to the length of the flow path (i.e. constant Pe). This can theoretically be shown to be the case if a single flow tube model should represent a network of flow paths with little mixing between the flow paths (see e.g. Rasmuson and Neretnieks 1981). In the case of a frequent mixing between the actual flow paths, theory predicts a dispersion coefficient independent of the accumulated distance in the flow direction and a Pe increasing with migration distance.

Assessment codes, such as the FARF31 used in SR 97 usually require constant transport parameters along the entire stream tube. This is in contradiction to the dispersion length increase with distance. One method which has been applied for determining effective Peclet numbers for cases with a varying flow field is the additive variance method (Neretnieks and Rasmuson, 1984). The method is based on the assumption that the variance in travel time may be integrated along the travel path. A calculation using the average flow velocity and the effective Peclet number should give similar results as when using a constant dispersion length and varying flow velocity. The effective Peclet number will depend strongly on the low water velocity parts of the stream tube. The approximation has been found to give good estimates of the effective Peclet number (Neretnieks and Rasmuson, 1984).

Evaluations of HYDRASTAR flow tubes (Elert *et al.*, 1998) using the correction of Neretnieks and Rasmuson (*op .cit.*), indicate that the effective Peclet numbers would only be a factor of 0.05 to 0.6 of the Peclet number derived assuming an average water velocity. However, the additive variance method as used in Neretnieks and Rasmuson assumes a constant dispersion length along the flow tube, where the value is assigned to give the expected spreading at the outlet. This may exaggerate the dispersion obtained in the low-flow part of the stream tube near the canister. Evaluations of HYDRASTAR flow tubes adding the variance in travel time, but assuming a dispersion length proportional to the migration lengths give Peclet numbers in the same order as obtained when using the average water velocity in the flow tube. Thus, the expected behaviour in fractured rock can be simulated by assuming a constant Peclet number when extrapolating the result of experiments to longer distances.

2.6 Scoping calculations

Elert *et al.*, (1998) have performed some scoping calculations with the FARF31 migration code (Norman and Kjellbert, 1990). Their results can be used to explore the applicability and the significance of the relations discussed previously in this chapter.

Figure 2.3 demonstrates that the breakthrough curves for sorbing species are invariant to the choice of a_w and t_w as long as the F-quotient is kept constant. This fact is also clearly demonstrated in the SKI project SITE-94, (SKI, 1996). Calculations by Elert *et al.*(1998) also show that sorbing migration through a series of segments of different F-quotients can be combined into a single segment with an F-quotient equal to the sum of the individual F-quotients.

If sorption effects are negligible, the F -quotient alone is not sufficient to describe the transport. Then t_{tot} is also needed as an effective parameter since the approximation of equation 2.3 is no longer valid. Matrix diffusion may to some extent be important also for non-sorbing radionuclides. However, scoping calculations carried out by Elert *et al.*, (1998) indicate a minor importance of this effect, given the low diffusivity of the rock matrix. At any rate, cases with non-sorbing tracer are usually of less importance in Performance Assessment. There, non-sorbing retardation is usually insignificant since many of the important nuclei either are strongly sorbing (such as the transuranic elements) or have very long half lives (as for ^{129}I).

Figure 2.3 also shows that the Peclet-number is far less important than F for sorbing species, at least for Peclet numbers larger than 2. At Peclet numbers higher than 50 the spreading effect of matrix diffusion and sorption will completely dominate the shape of the release at the outlet. For Peclet numbers higher than 100 dispersion will have no effect on the release from the geosphere.

The question also arises on how to combine segments with different Peclet-numbers. Based on scoping calculations Elert *et al.* (1998) suggest that the Peclet numbers in individual segments should be weighted against the F-quotient. By doing this, a single FARF31 solution coincides with a FARF31 solution made up of a series of segments, but the solution may still not necessarily match the actual dispersion behaviour in nature. However, as Pe at any rate is insignificant in relation to F for most performance assessment application this issue is of secondary importance for SR 97, but further exploration may be an interesting research option.

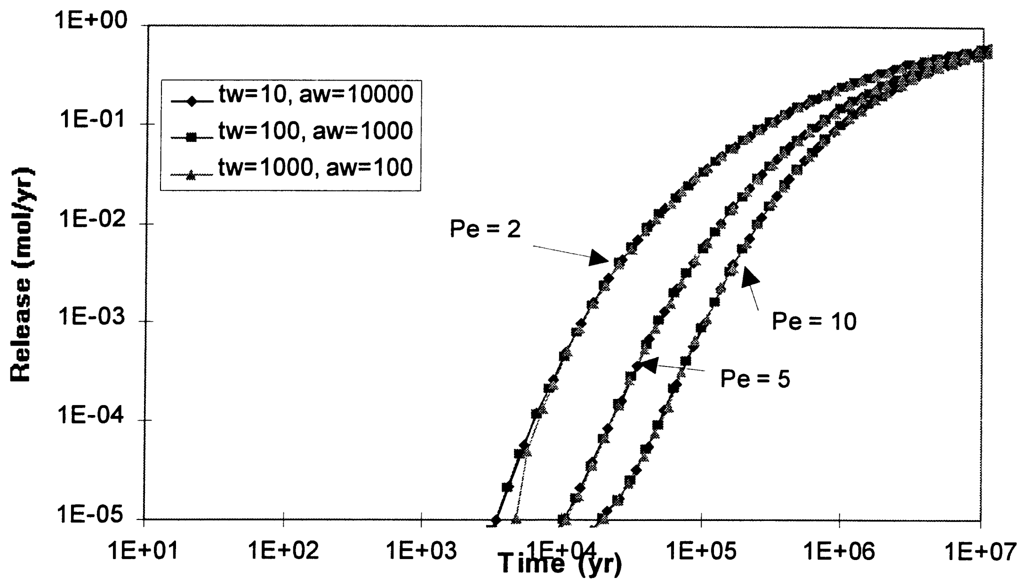

Figure 2.3: Simulations with FARF31 showing that the F-quotient and Pe-numbers control release for sorbing species whereas individual values of a_w and t_w have almost no impact. K_d=0.1

2.7 Conclusions

The issue regarding matrix diffusion in a single fracture cannot be resolved without further studies. Such studies are highly recommended. SR 97 would need to apply a rather conservative view on this issue, but research on the migration in a single fracture with spatially varying velocity fields is recommended.

The evaluation of matrix diffusion for a sorbing species along spatially varying flow paths clearly shows that the sum of the F-quotient in individual segments can be used as an effective F-quotient for the entire migration path. Generally both the F-quotient and t_{tot} are needed to describe transport. For sorbing species, the F-quotient alone is by far the most important parameter, whereas for non-sorbing species t_{tot} essentially describes the transport. Additional studies may be needed to fully clarify under which conditions the F-quotients are additive, but the approximation, if any, is regarded quite minor and will be acceptable for SR 97.

Further background work may be needed on the issue of dispersion. However, the multiple stream tube approach adopted implies that within each tube the dispersion term only needs to capture the variability of t_{tot} and F_{tot} *within* the tube. The variability *between* tube is taken care of by using multiple tubes. Furthermore, the Peclet number is far less important than the F-quotient for sorbing species, at least for Peclet numbers larger than 2. At Peclet numbers higher than 50 the spreading effect of matrix diffusion and sorption will completely dominate the shape of the release at the outlet. For Peclet numbers higher than 100 dispersion will have no effect on the release from the geosphere.

3 Field information and parameter estimates

This section identifies the need for site specific information on flow related migration parameters. It explores generic information on these parameters and its examines the existing experimental data from Aberg, Beberg and Ceberg which could be used to estimate these parameters. Finally, estimates of the parameters for use in SR 97 are suggested.

3.1 Hydrogeologic data

Hydrogeologic information provides input to the detailed hydrogeological models and is thus essential for the source term and migration modelling. The hydraulic information is used to estimate the spatial variability in hydraulic conductivity, fracture transmissivity distributions or channel conductance distributions for the stochastic continuum, discrete fracture network and channel network models, respectively.

Walker *et al.* (1997) assemble the available information from Aberg, Beberg and Ceberg for use in SR 97 and suggest parameters for the stochastic continuum models. Additional data (on fracture statistics) is needed for the discrete network modelling. In SR 97 such modelling will only be performed for Aberg. Relevant fracture network information for Aberg can be found in Uchida *et al.* (1997) and Follin and Hermansson (1996). For Beberg the discrete network model of Geier and Axelsson (1991) may be used. Recommendations for the proper use of these data lies outside the scope of this report and is not further discussed here.

3.2 Flow wetted surface per volume of rock

As discussed in chapter 2, migration in the far field to a large extent is controlled by the F-quotient being a function of flow and flow wetted surface. The flow part of F (either q or t) is predicted with detailed flow models, but additional field information is needed for the estimates of the flow wetted surface (a_w or a_r). In addition, it is essential to capture the correlation between flow and flow wetted surface in order not to bias the estimation of F.

Neither a_w nor a_r are material properties. However, estimates of a_w needs to be consistent with porosity assumptions made when predicting t_{tot}, which may lead to an unjustified attention to flow porosity. Estimates if a_r needs to be combined with estimates of the Darcy velocity q along the flow path in order to determine proper F-values. In a strongly varying flow field this may not be straight forward. Still, global estimates of a_r should be more stable than global estimates of a_w since a_r essentially only depends on the frequency and width of flow paths and q is the primary parameter solved for in hydraulic models, whereas a_w and t_{tot} also depend on the highly unknown and variable aperture distribution.

There are five potential sources for estimates of the flow wetted surface; "generic data", evaluation of tracer tests, geologic information, estimation of conductive fracture frequency directly from hydraulic tests and estimation from hydrological modelling. The usefulness and resulting estimates from these different sources are discussed in the following.

3.2.1 Generic information

Various experimental and theoretical methods have been used to obtain estimates of the flow wetted surface (Elert, 1997). Table 3.1 gives a summary of the flow wetted surface estimated by various methods. There is a large variability in the values depending both on the type of method used and on the characteristics of the rock. Furthermore, there is no assurance that the tracer tests actually showed any matrix diffusion effects. The estimates for the rock mass span four orders of magnitude (0.001-10 m^2/m^3 rock). The variability in the values for fracture zones is almost as high, 3.5 orders of magnitude (0.03 - 92 m^2/m^3 rock).

Table 3.1: Summary of estimates of the flow wetted surface (from Elert 1997).

Method	*Flow wetted surface per volume of rock a_r [m^2/m^3]*	*Flow wetted surface per volume of water a_w [m^2/m^3]*
Tracer experiments [Abelin *et al.* 1987]	0.2 - 2 (possibly up to 20)	
Tracer tests in fracture zone [Birgersson et al 1992]	5 - 23	
Tracer injection and borehole radar in fracture zone [Andersson et al, 1989b]	1.8	
Tracer test in fracture zone [Gustafsson and Nordqvist, 1993]	1 - 92	1180 - 8700
Observations of channels at Kymmen tunnel [Moreno and Neretnieks, 1991]	0.006 rock mass 0.03 zones	
Observations of channels at SFR [Moreno and Neretnieks, 1993]	0.017	
Observations of channels at Stripa [Moreno and Neretnieks, 1993]	0.2	
Bore hole measurements at Stripa [Moreno and Neretnieks, 1993]	0.4	
Observed area of site-scale structures [Voss et al, 1996]	0.12	
Uranium content and radon concentration [Glynn and Voss, 1996]	0.31 - 3.1	3100
Heat transport in rock [Nicol and Robinson, 1990]	0.05-0.08	
DFN-model calibrated to field experiment [Dverstorp, 1991]	0.001 - 5	
Discrete feature model [Geier, 1996]	0.01 - 0.1	
DFN-model [Nordqvist et al, 1996]	0.1 - 10	
LPT2 using equation 4.1 [Gylling et al, 1994)	1.2	

Table 3.1 shows that estimates of a_r in different crystalline rock assessments vary in the interval (0.01 m^{-1} - 10 m^{-1}), with 0.1 m^{-1} as a typical value. A priori it seems that this range (and "typical" value) would be the option also for SR 97. On the other hand it should be understood that the estimates have been made under various assumptions. Part of the range may in fact be regarded as modelling artefacts or at least general uncertainty rather than representing variability between different sites or migration paths.

Parameter values used for the flow wetted surface in performance assessment studies have been based on estimates made using a variety of methods. In most studies a range of values have been used, spanning 1-2 orders of magnitude. The proposed ranges generally overlap with a lowest value used in a safety assessment of 0.01 m^2/m^3 of rock and a highest value of 2 m^2/m^3 rock. In two recent performance assessment (TVO-92 and SITE-94) focus has been put on the quotient between the flow wetted surface and the water flux (F-quotient= $a_r L/q$). In Table 3.2 a summary of F-quotients from different assessments is given. For the other safety assessments the F-quotients have been calculated from the far-field parameters.

Table 3.2: Summary of F-quotient (a_rL/q) used in various safety assessments (from Elert, 1997).

Study	a_r	*L [m]*	*q [m³/(m²,a)]*	*F-quotient[a/m]* Low	*Reference*	*high*
KBS-3	0.4	100	10^{-4}		$4\cdot10^{5}$	
SKB 91	0.1	a)	10^{-3} b)	10^{4} c)	10^{5} d)	10^{7} e)
Project 90	0.01, 1	200	10^{-4}, 10^{-2}	$2\cdot10^{2}$	$2\cdot10^{4}$	$2\cdot10^{6}$
TVO-92	0.04-2 f)	400 f)	10^{-4} - 10^{-2} f)	$4\cdot10^{3}$	$2\cdot10^{4}$	$1\cdot10^{5}$
Kristallin-I	0.0024-0.066	200	$2.4\cdot10^{-5}$		$2\cdot10^{4}$	$5\cdot10^{5}$
SITE-94	0.01,0.1, 1 g)	500	10^{-5} - $2\cdot10^{-2}$	$7\cdot10^{2}$	$7\cdot10^{4}$	$6\cdot10^{6}$

Notes a) not evaluated, most frequent groundwater travel time was 100 years, b) median flux at repository level , c) assuming a groundwater travel time of 10 years, d) assuming a groundwater travel time of 100 years, e) assuming a groundwater travel time of 10000 years, f) F-quotients chosen from an analysis of different flowpaths from the repository, g) only used for the stochastic continuum modelling

3.2.2 Tracer tests

In theory tracer tests would be very important data. Gustafsson and Nordquist (1993) report of a range of 1 - 92 (m^{-1}) for Beberg resulting from evaluation by 12 different modelling teams of non-sorbing tracer test in the fracture zone 2. As of yet no tracer test based estimates of a_r have been presented for Aberg. As discussed by Elert (1997) the reported tracer tests from Aberg and Beberg are, however, not very sensitive to the flow wetted surface and should thus not be given a strong weight in the determination of the flow wetted surface. There may also be competing mechanisms, such as diffusion into fracture gauge, which would further complicate the interpretation of the test results. Furthermore, the Beberg value concerns the conductor zone 2 and gives no information in properties in the remaining rock mass.

In the ongoing and planned sorbing tracer tests within the first stage of the Tracer Retention Understanding Experiment (TRUE) at the Äspö Hard Rock Laboratory, matrix diffusion may possibly be an observable process (Andersson *et al.* 1997; Selroos and Cvetkovic, in press). In later stages of the TRUE, mass transfer mechanisms including matrix diffusion will be studied in more detail (Bäckblom and Olsson, 1994). An evaluation framework for sorbing tracer tests has specifically been developed within the TRUE project with the purpose of identifying parameters governing matrix diffusion (Cvetkovic and Selroos, in press).

3.2.3 Geological information

Glynn and Voss (1996) suggest to use the relation between the ^{222}Rn content of the groundwater and the uranium content in the rock as a measure of the flow wetted surface. They obtained an average area of 3 100 m^2 per m^3 of water. Given a porosity variation between 10^{-3} and 10^{-4} this would imply an a_r in the range of 0.3 - 3 m^2 per m^3

of rock. The authors note that the estimate involves several uncertain assumptions, but it is of interest to see whether independent methods yield results in the same region.

Mazurek *et al.* (1996) have made a detailed geological characterisation of water conducting fractures in the Äspö tunnel. However, apart from measurement of matrix porosity, the work in its present form seem to be of little relevance for estimating flow wetted surface or retention properties since derivation of hydrological and chemical parameter values for transport were not considered. However, their characterisation is potentially useful as it may provide a realistic geometry for describing matrix diffusion and the interchange between flowing and stagnant part of the fracture. More useful conclusions may possibly be drawn from future development of the work if it aims at including hydrological and chemical properties, including evidence of past matrix diffusion, of the studied fractures.

3.2.4 Hydraulic tests and conductive fracture frequency - CFF

Gylling *et al.*, (1994) suggest that a spatial average of the flow wetted surface per volume of rock could be estimated from the frequency of conductive fractures along a borehole. Using the theory of geometrical statistics (see e.g. Santaló, 1976) Gylling *et al.* (1997) show that:

$$\langle a_r \rangle = 4/H = 4 \cdot CFF \tag{3.1}$$

where $\langle a_r \rangle$ is an estimate of a_r and H is the "mean distance between channels intersected by borehole". Evidently H is the inverse of the conductive fracture frequency. Equation (3.1) assumes random fracture orientations, whereas in general $\langle a_r \rangle = 2C_p \cdot CFF$, where C_p is function of fracture orientation distributions and borehole orientation (Dershowitz, 1985). Furthermore, $\langle a_r \rangle$ estimated this way exactly equals (twice) the conductive fracture intensity (P_{32c}) used to describe the amount of fractures in discrete fracture network models, i.e.:

$$\langle a_r \rangle = 2 \cdot P_{32c} \tag{3.2}$$

counting the two sides of the fracture. The following can be noted:

- Both equations provide an average estimate of a_r and this average estimate does not contain any information on the correlation between a_r and the flow. Real migration paths may thus experience different fracture surfaces. Studies of such correlation could in fact only be made in a discrete model (ideally supported by experimental results).

- Both equations provide estimates of the actual conductive area of fractures (i.e. do not include the non-conductive paths) as long as the conductive parts have a convex form. The equations do not, however, consider variability in the conductivity and cannot be used to evaluate the more extreme channelling effects inside a fracture. This again means that the equations may overestimate a_r.

- The correction factor C_p is usually quite close to 2 (see e.g. Dershowitz *et al.*, 1996b) or Geier and Axelsson (1992), but P_{32c} is a more general measure than CFF and could also be estimated from the length distributions of traces from fractures judged to be conductive intersecting outcrops or tunnel walls (see e.g. Follin and Hermansson, 1996).

Provided estimates of CFF or P_{32c} could be obtained the equations still offer one of the few possibilities to obtain meaningful estimates of a_r as there is little other data available.

Gylling *et al.* (1994) suggest to underestimate the CFF from double packer hydraulic tests by assuming that each packed off section with a hydraulic conductivity above zero (or above a threshold) contains at least one conductive fracture i.e.

$$\langle CFF \rangle = \text{number of conductive test sections/ total section length} \tag{3.3}$$

The advantage of this idea is that it underestimates CFF and that estimates can be made from any site with packed off sections. The main disadvantage is that the result will depend on the test section length and the threshold value selected. Particularly the test section length dependence is quite severe. For 3 m sections the maximum CFF possible with equation 4.3 is 0.33 and for 25 m section the maximum CFF possible is 0.04.

Equation 3.3 has been applied to the three different sites in SR 97 using the hydraulic conductivity distributions assembled by Walker *et al.* (1997). Table 3.3 lists the resulting values of the CFF and the a_r estimates using equation 3.1. The table also lists CFF estimates of Aberg made by Gylling *et al.* (1994). For Aberg and Beberg the test section is 3 m and the conductive threshold has been $\log_{10}(K) = -9.71$. For Gideå (Ceberg) the test section length is 25 m and the conductive threshold has been $\log_{10}(K)=-10.25$. Estimates are made for Conductive Domains and Rock domains using the notation by Walker *et al.* (1997). For comparison table 3.3 also contains CFF and a_r estimates based on the 30 m tests at Äspö (Aberg) and the 20 m tests at Finnsjön (Beberg). The following can be noted:

- There is not a great difference between conductive domains and rock domains.
- The Ceberg values are about one order of magnitude less than the 3 m Aberg and Beberg values. This low value is probably very much influenced by the test section length . Note that equation 3.3 cannot produce CFF values larger than 0.04 for Ceberg i.e. only twice the number in table 3.3. On the other hand the 30 m and 25 m tests from Aberg and Beberg respectively are much closer to their theoretical limits (0.033 and 0.05 respectively). Thus it appears that the CFF is smaller at Ceberg compared to the other two sites.
- The estimate by Gylling *et al.* (1994) results in a higher CFF, but they did not use exactly the same dataset and also assumed a lower threshold (around $\log_{10}(K)=-12$).

A more careful method of estimating fracture transmissivity distribution and conductive fracture frequency from packer test data has been developed within the framework of discrete fracture network analyses (OxFILET see e.g. Dershowitz *et al.*, 1995) using an approach adapted from Osnes *et al.* (1988). The method assumes that the net transmissivity of a conductive test section is equal to the sum of the transmissivities of the conductive fractures that intersect the tested section. A test section could be non-conductive either because it does not contain fractures or if intersecting fractures have transmissivities below a threshold value. The intensity and fracture transmissivity distributions are then estimated by finding the best match between the observed distribution of packer interval transmissivities and the distribution of simulated test zone transmissivities.

The OxFILET approach has been applied to Aberg and Beberg as also displayed in Table 3.3. Evaluation of the hydraulic data from the TRUE-1 experiment at Äspö (Winberg ed., 1996) resulted in a CFF = 1.72 and an estimated P_{32c}, estimated by modelling, of 3.17, resulting in $<a_r>$=6.3. The CFF estimated this way is close to a CFF estimated by an attempt to geologically identify the conductive fractures, which resulted in a CFF = 1.55. Estimating the CFF instead using equation 3.3 yields a CFF of 0.26 (41 conductive sections/the total tested section length), which indicates that the difference between the CFF given by Winberg (ed., 1996) and the values reported above concern the estimation method rather than differences in data. Geier and Axelsson (1991) applied the OxFILET approach to the Beberg data, which resulted in a CFF=0.72 and a P_{32c} =1 m^{-1} (i.e. $<a_r>$=2 m^{-1}).

By mapping fracture traces on the TBM tunnel of Äspö (Aberg) Follin and Hermansson (1996) estimate a P_{32c}=0.2 m^{-1}, (i.e. $<a_r>$=0.4 m^{-1}). It is clear from the mapping procedure that only prominent fractures where included, indicating an underestimate of P_{32c}.

In the framework of SKI SITE-94 Voss *et al.* (1996) estimated the surface area of the SITE-94 structural model, which describes the distribution of the main conductors outside the repository area. The resulting P_{32c}=0.065 corresponding to $<a_r>$=0.12 is evidently an underestimate since Voss *et al.*, (1996) note that more than 30% of the flow occurs outside this structural model.

3.2.5 Discrete fracture network modelling

The main disadvantage with the use of equations 3.1-3.2 is that they do not describe the correlation between flow and surface area. *Assuming flow to be evenly distributed in all fractures is a strong simplification.* One possibility to study this correlation is through the use of discrete fracture network codes, which also is planned for SR 97 (see also chapter 5).

In SKI SITE-94 Geier (1996) performed particle tracking in a discrete feature model adopted to Äspö and then calculated migration paths surface areas weighted by the mass of solute within each element for a steady state source. The resulting estimates of a_r was in the range of 0.01 - 0.1 m^{-1}. This low range can be taken as an indication that the a_r values based directly on the P_{32c} values are too small, but may also be attributed to the weighting procedure since Geier (1996) weight the area with the fracture segment volume i.e. $W_i e_i L_i$ rather than with residence time suggested by equations 2.7 - 2.9 of this report. However, it is pointed out in SITE-94 (SKI, 1996) that the a_r estimates includes an arbitrary selection of averaging volume, which implies that a_r estimates alone are of very little relevance. Only F-quotient estimates are meaningful since they do not directly depend on the size of the averaging volume.

3.2.6 Conclusions

Table 3.3 compiles the reference to sources and suggested estimates of a_r discussed previously. For reason explained above it appears that the most defensible means of estimating a_r would be through estimates of CFF and P_{32c}. The a_r estimated by equation 3.1 or 3.2 is probably an overestimate of the "effective" a_r considering the correlation between flow and flow wetted surface as indicated by the discrete network analyses conducted by Geier (1996). On the other hand equation 3.3 underestimates CFF.

Table 3.3: Estimates of a_r (m^{-1}) at the SR 97 sites using different methods and data sources

Method	Reference	Aberg	Beberg	Ceberg
Tracer test				
Calibration with transport models	Gustafsson and Nordqvist (1993)		1-92	
Geochemical				
^{222}Rn U ratio	Glynn and Voss (1996)	0.31 - 3.1	n.a.	n.a.
Hydraulic data				
25 m test (eq 4.3) Rock	data from Walker *et al.* (1997).	n.a.	n.a.	0.08 (CFF=0.02)
25 m test (eq 4.3) Conductors	data from Walker *et al.* (1997).	n.a.	n.a.	0.1 (CFF=0.023)
30 m test (eq 4.3) all domain	data from Rhén ed (1997)	0.12 (CFF=0.03)		
20 m test (eq 4.3) all domain	data from Andersson J.E. *et al.*, (1991)		0.2 (CFF=0.05)	
3m test (eq 4.3) Rock	data from Walker *et al.* (1997).	0.6 (CFF=0.14)	1.2 (CFF=0.29)	n.a.
3 m test (eq 4.3) Conductors	data from Walker *et al.* (1997).	0.8 (CFF=0.2)	1.2 (CFF=0.32)	n.a.
3m test (eq 4.3) but different cutoff	Gylling *et al.*, 1994	1.0 (CFF=0.25)		
P_{32c} from OxFILET and TRUE I data	Winberg ed., 1996	6.3		
P_{32c} from OxFILET	Geier and Axelsson (1991)		2.0	
Mapping fracture traces on TBM-tunnel, estimate of P32c	Follin and Hermansson (1996)	0.4		
P_{32c} from surface area in SKI SITE-94 structure model	Voss et al., (1996)	0.12		
Modelling				
Back-calculated from DFN-model	Geier, 1996	0.01 - 0.1		

Inspecting table 3.3 suggest that a value of a_r in the order of 1 appears reasonable for Aberg and Beberg. An uncertainty range of a factor of 10, in both direction could be motivated by the underestimate of CFF illustrated by the OxFILET values on one hand and the correlation between flow and flow wetted surface as indicated by the discrete network analyses conducted by Geier (1996) on the other hand. The ranges are not in conflict with the very uncertain estimates from tracer tests or geochemical information. For Ceberg the only estimates are based on CFF estimated by equation 3.3. The resulting a_r value is most likely affected by the test section length and shorter test sections would most likely produce a higher CFF. On the other hand the number of non-conductive 25 m sections are high at Ceberg in comparision to the other sites, and in addition there are no other estimates. Consequently it is suggested to use 0.1 with an uncertainty range of a factor of 10 for Ceberg, while still noting that the rationale for this suggestions is very weak. Table 3.5 summaries these suggestions.

3.3 Estimates of flow porosity

Estimates of flow porosity could really only be made from tracer tests. Table 3.4 lists tracer test conducted at Äspö (Aberg) and Finnsjön (Beberg) together with estimates of ε_f. No tracer tests have been conducted at Gideå (Ceberg). The table builds on the compilation of tests by Andersson (1995). The estimates of flow porosity are made with simple analytical relation (using breakthrough time and flow) or by modelling the tests (see Andersson, 1995). Many of the tests have been analysed by multiple modelling teams within the Äspö Task Force and INTRAVAL exercises.

The table shows that flow porosity estimates seem to vary quite significantly in the range 10^{-4} to 10^{-1}. The higher value may possibly be attributed to Conductor Domains (see Walker et al., 1997) since the majority of tracer tests at Beberg have been conducted in the zone 2. The Aberg results suggest that rock mass flow porosity may be an order of magnitude less (i.e. 10^{-4}) than fracture zone flow porosity. Furthermore, Rhén ed. (1997) notes that the flow porosity at Äspö (Aberg) appear to be correlated with the hydraulic conductivites. (He shows linear regression between flow porosity and estimated hydraulic conductivity in log-log scale). A migration model should ideally match these general findings, which seems generally plausible, even if the information as such seems to be insufficient to provide estimates of F.

Inspection of table 3.4 suggests that a median value of the flow porosity, both at Aberg and Beberg is 10^{-3}. The range is large as can be noted from table 3.4 but is also a result of spatial variability and not pure uncertainty. Given the fact that the value chosen for the flow porosity has not effect on the calculated migration of sorbing radionuclides with FARF31 provided a_r is kept at desired values it is suggested to only use 10^{-3} in the geopshere migration calculations (FAR31). (For non-sorbing radionuclides the retardation is of little significance anyway). For the near-field release (i.e. in COMP23) the impact of porosity is larger and spatial variability manifest itself as uncertainty. Here one may consider 1 order of magnitude uncertainty. Lacking other information it is suggested to use these values at Ceberg as well. Table 3.5 summarises these recommendations.

Table 3.4: Tracer test conducted at Äspö (Aberg) and Finnsjön (Beberg) together with estimates of ε_f.

Site	Object and scale	Estimate of ε_f	Description and scale	Reference
Aberg	Zone	$1.3\cdot10^{-4}$ - $5.9\cdot10^{-2}$	Converging flow. 100-300 m	Gustafsson *et al.* 1992
Aberg	Rock mass	$1.8\cdot10^{-4}$	Detailed scale < 5 m	Winberg (ed.), 1996
Aberg	Rock mass	$0.9\cdot10^{-4}$ - $1.2\cdot10^{-4}$	Detailed scale < 5 m radialy converging	Andersson (1997)
Aberg	Rock mass	$1.2\cdot10^{-4}$ - $5.2\cdot10^{-4}$	Detailed scale <5 m, dipole flow	Andersson *et al.*, (1997)
Beberg	Zone	$8\cdot10^{-4}$ - $1.2\cdot10^{-2}$	Radialy converging flow. 155-189 m	Andersson *et al.* (1989a)
Beberg	Zone	$8\cdot10^{-3}$ - $6\cdot10^{-2}$	Transport of labelled drilling fluid from drilled borehole to water supply well. 440 m	Gustafsson *et al.* (1991)
Beberg	Zone	10^{-2}	Recirculating dipole flow. 155 - 220 m	Andersson *et al.* (1993)
Beberg	Zone	$4\cdot10^{-4}$ - $3\cdot10^{-1}$	Radially converging flow. Sampling over the entire thickness of the zone. 155-220 m	Gustafsson and Nordquist (1993)
Beberg	Rock mass	$7.9\cdot10^{-4}$ - $8.8\cdot10^{-4}$	Radially converging flow. 30 m	Gustafsson and Klockars (1981)

3.4 Estimates of fracture apertures

Locally the flow wetted surface per volume of water is inversely proportional to the aperture, but as pointed out in section 2.2, aperture cancels out when estimating the F-quotient. (They are only important indirectly as they determine the local ”transmissivity” of the fracture and hence the flow distribution). Consequently aperture estimates based on porosity estimates from tracer test cannot be used to estimate the flow wetted surface per volume of rock. However, estimates of aperture distribution in individual rock fractures, i.e. as measured by Hakami, (1995), are potentially useful for modelling the development of the flow wetted surface in a single fracture as the aperture distribution then can be used also to determine the flow distribution in the plane (see section 2.1). Even if the representativity of the fractures analysed by Hakami could be questioned, research in this direction making use of fracture aperture data is suggested but would not directly impact suggestions for transport parameters for SR 97.

3.5 Peclet number

A pragmatic approach of handling dispersion in multiple paths would be to acknowledge that competing ideas on dispersion models clearly exist, but given the relative unimportance of the dispersion for the radionuclide migration it may be treated as an uncertain macro-parameter. Literature data of Peclet-numbers fall within the range 2 to 40 (Elert *et al.,* 1992). At present there is no experimental basis for defining separate dispersion coefficients for the "good rock" or for fracture zones. It is not meaningful to try to estimate Pe-numbers site specifically. Following the discussion in chapter 2 and the estimates discussed it is suggested to use a Peclet number 10 as a best estimate and a range of 2 - 50. Table 3.5 summarises this recommendation.

3.6 Properties of the rock matrix

Data on matrix diffusivities, porosities and K_d-values are covered in other reports within SR 97. Carbol and Engkvist (1997) provide K_d-values and Ohlsson and Neretnieks (1997) cover diffusivities and matrix porosity. The matrix properties will not be further discussed in the present report.

3.7 Suggestion for parameters to be used in SR 97

Table 3.5 displays the suggestions for flow related transport parameters for use in SR 97 with best estimate and range. Motives for these suggestions are provided in the preceding sections. One should note that the ranges are quite speculative.

Table 3.5: Suggested flow related transport parameters for use in SR 97 with best estimate and range. One should note that the ranges are quite speculative.

Type of data	*Aberg*	*Beberg*	*Ceberg*
Flow wetted surface - a_r (m^{-1})			
All domains	1.0 (10 - 0.1)	1.0 (10 - 0.1)	0.1 (1. - 0.01)
Flow porosity ε_f			
All domains	10^{-3} (10^{-4} - 10^{-2})	10^{-3} (10^{-4} - 10^{-2})	10^{-3} (10^{-4} - 10^{-2})
Pe-number			
All domains	10 (2-50)	10 (2-50)	10 (2-50)

In addition the following can be noted:

- Only limited data exist within SR 97 for direct estimates of the flow wetted surface. In future development there is reason to explore for other sources of information.

- There is currently no clear experimental support for assigning different values of a_r to different parts of the rock (such as major discontinuities and the rock between these discontinuities). There is probably such a correlation for flow porosity (ε_f), but given the present incapability of properly handling varying flow porosity in assessment codes (see chapter 5) a single value is still suggested for SR 97. More precise parameter estimates would be needed to further substantiate such a conclusion and proper means of handling it would need to be developed before it could be considered in performance assessment.

- Estimates of F-quotients (or complete input data sets to FARF31) from alternative models appear to be an important complement to the direct estimation of a_r. Such analyses are also planned within SR 97.

4 Input needs for the SKB assessment codes COMP23 and FARF31

In SR 97, SKB will apply a calculation chain for evaluating the release from the fuel, migration through the near-field, migration through the far-field and biosphere doses using different component models. Evaluations and evaluation tools leading up to parameters to COMP23/FARF31 have to adopt to the possibilities of these codes.

4.1 Input to COMP23

The source term code COMP23 is essentially equivalent to the NUCTRAN code (Romero *et al.*, 1995). COMP23 (and NUCTRAN) considers release through different pathways from the canister deposition hole. COMP23 requires the following input:

- the geometry of the system,
- q_1 and ε_{f1} - the groundwater darcy velocity (i.e. $L^3T^{-1}L^{-2}$) and flow porosity in a fracture intersecting the canister deposition hole,
- q_2 and ε_{f2} - the groundwater darcy velocity and flow porosity in the disturbed zone
- q_3 and ε_{f3} - the groundwater darcy velocity and flow porosity in a fracture zone intersecting the tunnel backfill
- q_4 and ε_{f4} - the groundwater darcy velocity and flow porosity in a fracture zone close the deposition hole, but not intersecting it.

These parameters are used to estimate ”equivalent flow” rates for these four potential release pathways as further discussed by Moreno and Gylling (1998). However, in the current conceptualisation of the code only the darcy velocity of the deposition hole (q_1) is obtained from the groundwater flow solution, whereas the others are derived as different multiples of q_1. When using input from HYDRASTAR (Norman, 1992), q_1 represents an average over the cell size, which usually is around 30 m. 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 COMP23 assumes diffusion up to these paths. This means that the proper selection of q_3 and q_4 values is not very important and conservatively high values could be selected without biasing the function of the near-field. For consistency, however, it would indeed be desirable to include realistic estimates of these flows. Alternative scenarios may also change the relative importance of these flows.

An important assumption in the present conceptualisation of COMP23 is that migration in the tunnel backfill is driven by diffusion and not advection. It is not certain that there will be no groundwater flow in the backfill. In order to address this problem, Moreno

(1998) 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 a factor of two for a few nuclides.

Another issue worth commenting on is the potential correlation between near field flow and retention properties of the far-field migration paths. It seems to make sense that high *canister scale darcy velocity*, q_{nf}, should be correlated to low F values given that F depends on the inverse of the far-field darcy velocity. Exploring such a correlation would potentially be important for the total consequences but also for the potential gains of an active canister emplacement policy.

4.2 Input to FARF31

As already mentioned in chapter 2, the SKB approach to migration modelling is to divide the flow field into multiple single flow paths and to apply an advection-dispersion model (i.e. FARF31) to each path. The hydraulic input parameters to FARF31 are

t_{tot}	-	"conservative travel time"
$a_{w,glob}$	-	"flow wetted surface per volume of water"
Pe	-	"Peclet number"

The FARF31 results, for a given radionuclide with K_d-value and effective matrix diffusivity (D_e) fixed, essentially depends on

$F_{tot}=a_{w,glob}t_{tot}$, Pe and t_{tot}

where t_{tot} in itself is most important for non sorbing nuclides, whereas F usually totally controls the release of sorbing nuclides (see figure 2.4).

The discussion in chapter 2 addresses principles of how to assign effective parameters to individual paths also for the situation were the flow paths "properties" vary along the flow path. The discussion shows that, at least under specific conditions it is possible to define rules for how to derive "equivalent parameters".

The analysis of a general flow path in section 2.2 suggest that $F_{tot} = \Sigma F_i$ where $F_i=t_i a_{w,i}$ for segment *i*, as long as dispersion is not the dominating transport mechanism. This means that if selecting $t_{tot}=\Sigma t_i$ and $a_{w,glob}= F_{tot}/t_{tot}$, FARF31 will in fact produce the same matrix diffusion/sorption results as a code that takes care of individual segments. The question still arises how to select a proper value of F_{tot} in case the FARF31 flow tube is made up of several flow paths in the flow model. The precise application of these methods would need to be fitted to the actual flow model used for deriving the flow input, see chapter 5.

For selection of Peclet-numbers the pragmatic approach of chapter 3 should be applied. If there are multiple branching paths "inside" the modelled flow tube the minimum F_{tot} path within this tube should be selected to represent the path. A more ambitious approach, for models handling multiple and branching paths such as FracMan/PAWorks or CHAN3D (see chapter 5), would be to actually try to calculate the t_{tot} and F_{tot} distributions and then use these as input to a set of one-dimensional migration simulations with individually high Peclet-numbers. Evidently the result will also depend on the mixing conditions assumed at path intersections.

5 Derivation of input to COMP23 and FARF31 from detailed scale hydrological models

The groundwater flow modelling of SR 97 primarily serves as input to the assessment calculations. The approach adopts a stochastic continuum model, HYDRASTAR. In addition, discrete fracture network (FracMan/PAWorks) and channel network modelling (CHAN3D) are used in a few cases. This chapter discusses how these different codes could deliver input parameters to the assessment calculations.

5.1 HYDRASTAR

The main alternative for producing flow tubes (and flow paths) presently considered by SKB is the stochastic continuum model HYDRASTAR (Norman, 1992). Flow tubes to be used in FARF31 are produced by particle tracks, where particles are released from a set of release points covering the repository. However, a single particle track represents each release area (usually 30 x 30 m^2) and no random mixing between different paths is considered. This means that HYDRASTAR presently produces a single path for each flow tube.

5.1.1 Estimate of Darcy velocity at canister scale

The estimate of the Darcy velocity at the canister scale is simply taken from the HYDRASTAR model value. However, one should recognise that the block size usually used (i.e. 30 x 30 x 30 m^3) is larger than the scale of the deposition holes. The HYDRASTAR solution makes it possible to evaluate correlation between the near-field Darcy velocity and the properties of the far-field migration paths. Such a correlation should be studied as suggested in chapter 3.

5.1.2 Estimate $a_{w,glob}$ and t_{tot} from present version of HYDRASTAR

The present version of HYDRASTAR cannot handle varying values of the flow wetted surface along the flow path nor varying flow porosity. It should be noted that it would be incorrect to impose a varying flow porosity field as flow porosity is strongly correlated to the flow wetted surface per volume of water. Instead the following approach is suggested:

1. Select a (global) value of a_r = flow wetted area per volume of rock and a global flow porosity ε_f, (see section 4.6 and table 4.5) and calculate $a_{w,glob} = a_r/\varepsilon_f$
2. Calculate $t_{tot,k}$ for each flow path k in HYDRASTAR, *using the same flow porosity* ε_f as in step 1 (then $F_{tot,k} = a_{w,glob}(t_{tot})_k$).

5.1.3 Estimates of $a_{w,glob}$ and t_{tot} from developed version of HYDRASTAR

It has been discussed to develop HYDRASTAR such that it can handle spatial variability in flow porosity and flow wetted surface. In such a case FARF31 parameters should be estimated as follows:

1. Select a spatial distribution a_r and ε_f,
2. For each flow path calculate $F_{tot,i} = \{\int a_r(s)/q(s)ds\}_i$, and $t_{tot,i}=\{\int \varepsilon_f(s)/q(s)ds\}_i$,
3. Calculate $\{a_{w,glob}\}_i = F_{tot,i}/t_{tot,i}$

However, given the difficulties in estimating data as discussed in chapter 3 and the existence of the alternative approaches (FracMan/PAWork or CHAN3D) such a development is not recommended at this stage.

5.1.4 Multiple paths and the Peclet-number

The present way of abstracting flow tubes from HYDRASTAR to FARF31 does not include the possibility for multiple migration paths within the same flow tube. Consequently, from a practical point of view the problem of multiple paths does not need to be addressed. However, in terms of data it highlights the question whether the averaging scale used in HYDRASTAR would resolve the flow field to enough detail. This issue could possibly be highlighted by comparison with the results of the more detailed scale discrete fracture and channel network models. The recommended ”pragmatic” approach is to use the values of Pe suggested in table 3.5.

5.2 FracMan/PA-Works

A discrete modelling approach (e.g. as applied in FracMan/PA-Works, Dershowitz *et al.,* 1995, Foxford *et al.,* 1996) builds on the geometry of the conductive fractures and thereby both in itself provides estimates of a_r (need not be specified explicitly) and its correlation to flow. Thereby a DFN approach can directly produce estimates of F, without the intermediate stage of a_r, v_i and q. There are however several issues that needs to be addressed also for the DFN-approach. These include:

- representativity of the network (i.e. how well can you estimate the actual fracture network geometry from the limited measured information),
- assessment of the relevant area and details of transport in the plane of single fractures,
- derivation of ”global” estimates of input parameters to FARF31 from the DFN results.

The first issue is general to DFN-modelling and will not be discussed in this memo. The latter issues are elaborated below.

5.2.1 Estimate of Darcy velocity at canister scale

In Dershowitz *et al.,* (1998), the canister holes are assumed to have no net effect on the flow system - neither enhancing the flow along the holes, nor reducing the net flow. This is modelled by representing the canister holes by fractures with a transmissivity of 10^{-20} m^2/s, but not removing the connections through the canister holes. Clearly, this is not meant to imply that the fractures extending through the canister holes continue to exist even after the holes are constructed. However, if the canister holes do not influence the flow field, the flow through the canister holes would be re-routed into the portions of the fractures around the canister holes such that the net flux would be unchanged .

The input to COMP23 is calculated as follows. For each canister hole, PAWorks identifies pipes bringing flux to the canister hole, through the canister hole, and away from the canister hole. PAWorks calculates the sum of the flows away from the canister hole, as an approximation to the flow past the canister hole. In order to estimate the Darcy velocity this flow is divided by the cross sectional area of the canister deposition hole (i.e., approximately 10 m^2).

5.2.2 Estimate of F in a single fracture

Estimates of F_{tot} are to be based on estimates of F in the single fractures making up a flow path. Figure 5.1 displays a "typical" fracture, *j*, intersected by two other fractures. The figure also illustrated the concepts FWA_j and RSA_j used by Dershowitz *et al.* (1996b).

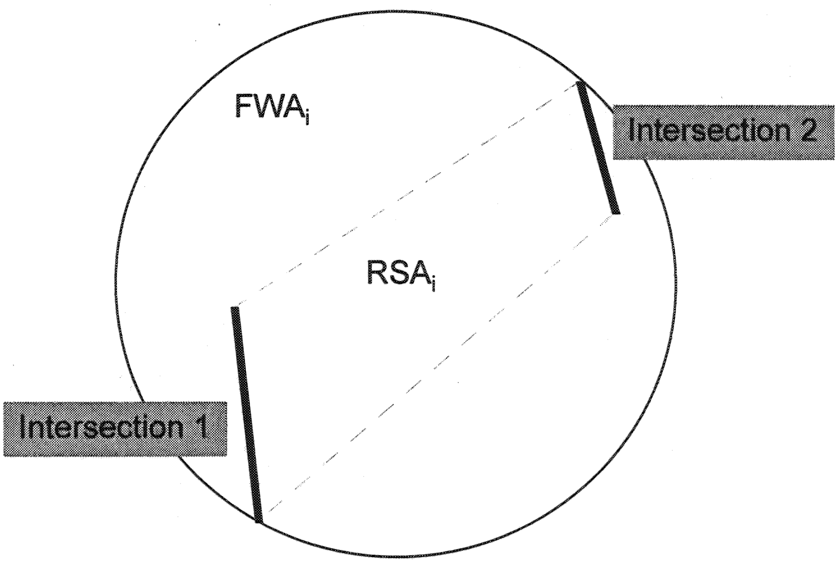

Figure 5.1: A single fracture with intersections in FRACMAN/PA-Works

In the fracture segment, PAWorks calculates t_j (travel time from intersection 1 to intersection 2) and F_j (local F-value) through the following relations:

$$t_j = RSA_j e_j / Q_j$$

$F_j = 2RSA_j/Q_j$

where Q_j is the flux (m^3/s) between the intersections and e_j the aperture. The equation implies that the entire RSA is available for matrix diffusion. The aperture is obtained from the segment transmissivity assuming:

$e_j = 0.5T^{0.5}$.

Evidently, the aperture formula is uncertain and questionable, but it should be recognised that these relations are consistent with the suggestions in section 2.2 of this report. The F-values do not depend on the aperture, but the assumption is made that the flow is evenly distributed over the entire RSA_j area.

5.2.3 Estimates of $a_{w,glob}$ and t_{tot}

In order to calculate "equivalent" FARF31 parameters from the PA-Works solution, one should derive the path from each (flowing) deposition hole i and along each path calculate :

1. $\{t_{tot}\}_i = \{\Sigma t_j\}_i$
2. $\{F_{tot}\}_i = \{\Sigma F_j\}_i$
3. $\{a_{w,glob}\}_i = \{F_{tot}/t_{tot}\}_i$

where j is fracture number along path i. Equivalent parameters for FARF31 for this deposition hole are then t_{tot} and $a_{w,glob}$.

In order to make meaningful comparisons with HYDRASTAR results, one should ensure that the input P_{32c} for the discrete network is consistent with the a_r value selected for the HYDRASTAR results. This consistency check is needed to make sure that potential differences between DFN-results and HYDRASTAR is due to the correlation between flow wetted surface and flow in the DFN model and not biased by different assumptions on P_{32c}.

5.2.4 Multiple paths from a single release point and the Peclet number

The FracMan/PAWorks model produces multiple paths from a single canister release point. In practice multiple paths could be handled by calculating t_{tot} and F_{tot} for each identified pathway. A proper distribution of t_{tot} and F_{tot} could be obtained by making the probability of selection of a path at branch to be proportional to the flux of the path. A direct approach to utilise this information for assessment calculations would be to produce a set of FAR31 solutions, with individually high Peclet numbers, but with t_{tot} and F_{tot} drawn from the distribution estimated in this way.

If this approach is not considered practical, the alternative approach would be to select a representative value of the calculated $\{t_{tot}, F_{tot}\}$ distribution (such as the mean, median or the mininum) combined with a low Peclet number to represent the spread. Clearly, the

Peclet number could be estimated from the t_{tot}-distribution, as was done in SKI SITE-94 (SKI, 1996). However, essentially the problem of finding correct dispersivities are the same as with HYDRASTAR. This means that the "pragmatic" approach described in section 5.1.4 may be applied here as well.

5.3 CHAN3D

One of the concepts behind the Channel Network model (see e.g. Gylling *et al.,* 1996) and the corresponding code CHAN3D is that flow and transport take place in channels in the rock. This is based on field observations from boreholes and tunnels. Most of the flow and transport take place in fracture zones. The fracture zones are represented by channels from a log-normal distribution with a mean value of the conductance (or conductivity) to match the measured transmissivity. The standard deviation in the conductance distribution is estimated from the measured hydraulic conductivity data. The rock mass is represented by channels taken from a distribution with a lower mean value in conductance. The same standard deviation as for the fracture zones is used.

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 regarding the numerical scheme, the channel network model is quite similar to an integrated finite difference model, but where the explicit channels facilitate particle tracking algorithms and allow to calculate the transport of solute that interact with the rock matrix (diffusion and sorption). 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).

5.3.1 Estimates of the Darcy velocity at canister scale

Estimates of the Darcy velocity at the canister scale are obtained by sampling the calculated flow at the canister scale. The resolution will evidently depend upon the resolution of the CHAN3D model.

5.3.2 Estimates of $a_{w,glob}$ and t_{tot}

For a given value of a_r CHAN3D calculates a "flow wetted surface" FWS in each channel using:

$$FWS_i = 2W_i \cdot L_i$$

$$W_i = a_{r,i} L^2/6$$

where W_i is the channel width, L_i the channel length and a_{ri} the specific flow wetted area for this channel. (The number 6 in the denominator stems from the fact that CHAN3D assumes channels around the 12 edges of the cube.) In practice, the channel length is constant throughout the model. Furthermore, since usually the specific flow-wetted surface, a_r, is estimated from fracture zone data, channels within the fracture zones are given a flow-wetted surface, FWS, based on a_r (i.e. $a_{ri}=a_r$) and channels in the rock mass are given a smaller flow-wetted surface, FWS. Partly based on field data and maybe somewhat arbitrary 10% of the value for fracture-zone channels is used by Gylling *et al.* (1996), i.e. $a_{ri}=0.1a_r$. It is possible to assign one individual FWS to each channel, but since no statistics for the distribution of a_r are available, one value of FWS is used for channels in the fracture zones and one value of FWS is used for the channels in the rock mass.

By assigning an FWS value for each channel and calculating the flow distribution in the channel network, it is possible to obtain an F-value for each channel. For each flow path from the repository to the release points, the individual F_i values may be added to a F_{tot}.

The approach to calculate the "equivalent" FARF31 parameters from the CHAN3D calculations is:

- Select an a_r from Table 3.5
- Calculate FWS_i as discussed above.
- Derive the transport paths from each canister of interest in the repository to the release points.
- For each transport path calculate:
    - $t_{tot,i} = \{\Sigma t_j\}_i$
    - $F_{tot,i} = \{\Sigma(FWS)_j/Q_j\}_i$
    - $a_{wi} = F_{tot,i}/t_{tot,i}$

where j ranges from 1 to the number of channels traversed along each path and Q_j is the flow rate (L^3T^{-1}) in path j. Equivalent parameters to FARF31 for a specific canister location is then t_{tot} and a_w.

5.3.3 Multiple paths from a single release point and the Peclet number

As for the discrete network approach CHAN3D produces multiple paths from a single canister release point and thus contains the probably most important dispersion mechanisms. In practice multiple paths are handled by calculating t_{tot} and F_{tot} for each particle track and thus producing distributions of t_{tot} and F_{tot}. A direct approach to utilise this information would be to produce a set of FAR31 solutions, with individually high Peclet numbers, but with t_{tot} and F_{tot} drawn from the distribution estimated by CHAN3D.

If this approach is not considered practical, the alternative approach would be to select a representative value of the calculated t_{tot}, F_{tot} distribution (such as the mean, median or the minimum) combined with a low Peclet number to represent the spread. Clearly, the

Peclet number could be estimated from the t_{tot}-distribution, as was done in SKI SITE-94, but for the same reasons as outlined previously the same approach as outlined in section 5.1.4 may be applied here as well.

6 Development projects

The previous chapters suggest pragmatic approaches to select values of the flow wetted surface and related parameters and how these should be utilised in the SR 97 assessment. Clearly, site specific estimates of these parameters could only be made within broad ranges. In order to improve assessment of migration parameters it is strongly recommended that special analyses are initiated, which may resolve some of the issues which now have to be treated with variations and conservative assumptions. The outcome of these analyses should also stimulate renewed efforts for site characterisation and measurement.

6.1 Single fracture

A study should be initiated with the aim to evaluate the fracture surface available for matrix diffusion including the effect of diffusion into stagnant zones. This evaluation can be performed at different levels, ranging over simple evaluations of relative resistance, numerical analysis of simplified fractures to studies of spatially averaging fractures. The relative importance of the diffusion path and the matrix diffusion path change with time. In order to more comprehensively resolve this problem, numerical simulations in a spatially varying fracture, for example, using the aperture distributions measured by Hakami (1995), under different flow regimes seems to be an important alternative. In addition, new data are underway from Hakami and Gale from the TRUE-1 pilot resin injection experiment (Winberg, personal comm.).

The study should preferably address the following combined issues:

- The study should explore to what extent the diffusion into stagnant or low flow parts of a fracture could appreciably increase the retardation of radionuclides both directly and increasing the accessible rock surface. The study should consider radionuclides with different sorption properties.

- The study should quantify the risk of misinterpreting diffusion into stagnant or low flow parts as matrix diffusion effects in short term migration experiments.

6.2 Migration modelling directly in the flow codes

It would definitely be of interest to check the correctness of the effective parameters derived using the relations in section 2.2. Among possibilities to explore the following may be considered:

- Alterations in HYDRASTAR to allow for spatial variation of the flow porosity and the flow wetted surface per volume of rock. Either for each model block or for separate values for different types of rock (good rock, zones). Integration of F-quotients along the stream tube.

- Integration of effective Peclet numbers along the stream tube including studies of the dispersion caused by multiple flow paths with different flow as well as with different flow wetted surface.

- Try to calculate the t_{tot} and F_{tot} distributions and compare the results with the pragmatic solution using the discrete fracture network or the channel network approaches discussed in chapter 5. The resulting distribution will also depend on the mixing conditions at the flow path "intersections". (If complete mixing is assumed the distribution should be flux averaged).

- Direct solution of the migration in discrete fracture networks, or in paths generated by PA-Works (e.g. using RIP, Miller, 1996).

- Direct solution of migration in the CHAN3D network.

6.3 Exploring further evidence of matrix diffusion

Given the significance of matrix diffusion, further efforts in the Äspö HRL TRUE experiments to actually try to determine matrix diffusion should be of high priority. Matrix diffusion will be a prime focus of the up-coming 2nd (detailed) phase of TRUE. Plans are also underway to conduct a "static" diffusion experiment in a packed off borehole section in a low permeable (matrix) environment at Äspö. It also appears warranted to continue the work for indirect geological evidence of matrix diffusion. Extension of the work of Mazurek *et al.* (1996) as discussed in chapter 4 is one important possibility.

7 Conclusions and recommendations

The evaluation made in this report should make it possible to select flow related transport parameters for the SR 97 safety assessment project. The derivation of efficient parameters is discussed, available field data are evaluated and suggestions are made on how to adjust input into a format suitable for the SR 97 assessment codes.

The evaluation of matrix diffusion for a sorbing species along varying flow paths clearly shows that the sum of the F-quotient in individual segments can be used as an effective F-quotient for the entire migration path. For non-sorbing species the F-quotient is not sufficient to describe transport as then the advective velocity determines migration times. Further background work may be needed on the issue of dispersion. However, the multiple stream tube approach adopted implies that the variability *between* tubes is taken care of by using multiple tubes. Furthermore, the Peclet number is far less important than the F-quotient for sorbing species, at least for Peclet numbers larger than 2.

The evaluation of generic data and of field data has resulted in estimates of flow wetted surface per volume of rock, flow porosity and Peclet-numbers to be used in SR 97. One should note that the ranges are quite speculative.

In conclusion, it is clear that site specific estimates of flow related migration parameters could only be made within broad ranges. In order to improve precision in these estimates, and thus potentially decrease uncertainty ranges in future assessments, both theoretical and experimental development is needed. It is strongly recommended that special analyses are initiated, which may resolve some of the issues which now have to be treated with variations and conservative assumptions. The following is suggested:

- develop the theoretical understanding of migration and matrix diffusion,
- study the effect of diffusion into stagnant or low flow zones in a single fracture,
- migration modelling directly in the flow codes,
- exploring for further evidence of matrix diffusion from tracer tests, static diffusion tests, geology and geochemistry.

This may potentially result in a better perspective on the flow wetted surface values actually selected and could also show a way further on how to reduce uncertainties in the estimates in coming performance assessments.

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