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Retention mechanisms and the flow wetted surface – implications for safety analysis

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RETENTION MECHANISMS AND THE FLOW WETTED SURFACE - IMPLICATIONS FOR SAFETY ANALYSIS

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This report concerns a study which was conducted for SKB. The conclusions and viewpoints presented in the report are those of the author(s) and do not necessarily coincide with those of the client.

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ABSTRACT

The purpose of this report is to document the state-of-the-art concerning the flow wetted surface, its importance for radionuclide transport in the geosphere and review various suggestions on how to increase the present knowledge. Definitions are made of the various concepts used for the flow wetted surface as well as the various model parameters used. In the report various methods proposed to assess the flow wetted surface are reviewed and discussed, tracer tests, tunnel and borehole investigations, geochemical studies, heat transport studies and theoretical modelling.

Furthermore, a review is made of how the flow wetted surface has been treated in various safety analyses: KBS-3, SKB-91, Project-90, TVO-92, Kristallin-I and SITE-94. The influence of the flow wetted surface on the results found in the various studies is summarized.

Finally, an overall discussion with recommendations is presented, where it is concluded that at present no individual method for estimating the flow wetted surface can be selected that satisfies all requirements concerning giving relevant values, covering relevant distances and is being practical to apply. Instead a combination of methods must be used. In the long-term research as well as in the safety assessment modelling focus should be put on assessing the ratio between flow wetted surface and water flux. The long-term research should address both the detailed flow within the fractures and the effective flow wetted surface along the flow paths.

SAMMANFATTNING

Syftet med denna rapport är att dokumentera kunskapsläget vad gäller den yta som är tillgänglig för matrisdiffusion och sorption i det sprickiga berget, den sk flödesvätta ytan, dess betydelse för transporten i geosfären samt granska olika förslag på metoder att öka nuvarande kunskap. De definitioner som används på flödesvätt yta och hur dessa används i olika modeller diskuteras. I rapporten görs en genomgång av olika metoder för att uppskatta den våta ytan, spårämnesförsök, undersökningar i tunnlar och av borrhål, geokemiska studier, värmetransportförsök och teoretiska modeller.

Vidare görs en genomgång av hur den flödesvätta ytan har behandlats i olika säkerhetsanalyser: KBS-3, SKB 91, Projekt 90, TVO-92, Kristallin-I och SITE-94. Den inverkan som den flödesvätta ytan har befunnits ha på resultatet sammanfattas.

Slutligen diskuteras det tidigare arbetet och rekommendationer för fortsatt arbete presenteras. Det slås fast att det för närvarande inte finns någon enskild metod som uppfyller alla krav som kan ställas på att ge relevanta resultat över relevanta avstånd och som även är praktisk att använda. Istället bör en kombination av metoder användas. Både för långsiktig forskning och för modellarbete i samband med säkerhetsanalyser bör tonvikten läggas på uppskattning av kvoten mellan flödesvätt yta och vattenflöde. Den långsiktiga forskningen bör inrikta sig på frågor som rör både det detaljerade flödet inom sprickor samt hur den effektiva tillgängliga ytan varierar längs flödesbanor och vilken rumslig variation som finns.

CONTENTS

1	Introduction	1
1.1	Background	1
1.2	Purpose and scope	1
2	Definitions of flow wetted surface	3
2.1	Specific flow wetted surface	4
2.2	Relation between flow wetted surface and water flux	5
3	Methods for determination of flow wetted surface	7
3.1	Tracer migration experiments	7
3.2	Tunnel observations	9
3.3	Borehole information	10
3.4	Fracture characterization	11
3.5	Geochemical effects	12
3.5.1	Red coloring of rock	12
3.5.2	Radon concentration in groundwater	12
3.6	Theoretical modelling	13
3.7	Heat transport and storage in rock	15
3.8	Discussion	16
4	Application of flow wetted surface in safety assessments	20
4.1	KBS-3	20
4.2	SKB 91	20
4.3	Project-90	21
4.4	TVO-92	22
4.5	Kristallin-I	23
4.6	SITE-94	24
4.7	Summary	28
5	Discussion and recommendations	32
6	Acknowledgements	34
	List of Notations	35
	References	36

1 Introduction

1.1 Background

Disposal of spent nuclear fuel in deep rock is based on the principle of multiple barriers: engineered barriers such as the canister and the backfilling material, and natural barriers such as the bedrock itself. The deep bedrock constitutes a barrier by providing a geologically stable environment and low water fluxes. Furthermore, many radionuclides interact with the mineral surfaces of the rock and are significantly delayed in their transport through the rock. For radionuclides with a radioactive half-life considerably less than the travel time in the geosphere, the release to the biosphere will be significantly reduced by this process. Investigations of radionuclide transport in crystalline rock have shown that matrix diffusion into the rock matrix and subsequent sorption on the inner surfaces of the rock is by far the most important retardation mechanism for sorbing radionuclides [Neretnieks, 1989].

The water flow in crystalline rock is very unevenly distributed. Only a part of the visible fractures carries any flowing water and only a few of these fractures are responsible for the largest parts of the observed flow rates. There is also evidence that the flow is located to limited pathways within the fractures [Neretnieks, 1987]. These are usually referred to as channels. The actual nature of the flow paths is important for the radionuclide transport for several reasons. Firstly, it determines the size of the contact area between the flowing water and the rock, a parameter that is crucial when estimating the extent of radionuclide sorption and retardation. Secondly, the flow path connectivity is of importance for the residence time distribution and thereby for the dispersion of radionuclides.

Thus a lot of effort has been put on understanding the nature of flow paths within crystalline rock and quantifying the size of the contact area between the water and rock, often referred to as the flow wetted surface. However, quantification of the flow wetted surface has proved to be difficult. A number of methods have been suggested on how to determine the flow wetted surface by combining theoretical methods and practical experiments, but so far no general consensus has been reached concerning suitable methods for measuring the flow wetted surface.

1.2 Purpose and scope

The purpose of this report is to document the state-of-the-art within this area and review various suggestions on how to increase the present knowledge. Various

definitions and modelling concepts for the flow wetted surface are described. A review is made of safety analysis studies where the effect of the flow wetted surface have been studied. A review is also made of proposals for methods to *determine the flow wetted surface*.

The report is disposed as follows:

- in Chapter 2 definitions are made of the various concepts used for sorption and the flow wetted surface as well as the various model parameters used.
- in Chapter 3 various methods proposed to assess the flow wetted surface are reviewed and discussed.
- in Chapter 4 a review is made of how the flow wetted surface has been treated in various safety analyses. The influence of the flow wetted surface on the results found in the various studies is summarized.
- and finally in Chapter 5 an overall discussion with recommendations is presented.

2 Definitions of flow wetted surface

The term flow wetted surface refers in this report to the parameter used to describe the contact area between the flowing water and the rock. Other names for this parameter are specific flow wetted area, flow wetted surface area, specific surface area, active surface, FWS, etc. Not only the terminology differs between different groups but also the way the parameter is defined, depending on the method used for estimation of the surface, the type of mathematical model it is used in and how it is parametrized in the mathematical model.

In a conceptual picture of flow in a fracture [Tsang and Tsang, 1987], flow occurs only in part of the fracture area (the channels), other parts of the fracture are filled with more or less stagnant water, while in the remaining part the fracture is closed, either because the rock surfaces are in contact or because of the presence of fracture filling material. Figure 2.1 gives a conceptual description of the flow wetted surface of an individual fracture. Parts of the fracture with a high flow rate in black, parts with intermediate flow in shades of gray, while the lightest gray shade illustrates parts with practically stagnant water. In Figure 2.2 a conceptual description is given of a flow path through a set of fractures. The figure illustrates the type of flow pattern that could be expected in a case with rock stresses in a preferential direction. In the first and last fracture, the flow is concentrated to channels, while in the middle fracture the flow is relatively evenly distributed over the fracture surface.

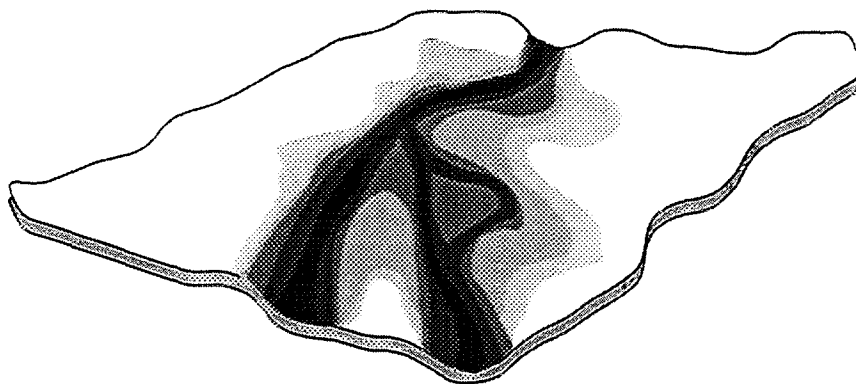


Figure 2.1 Conceptual description of flow paths in a fracture. Parts of the fracture with high flow rate in black, parts with intermediate flow in grey and parts with practically stagnant water in light grey. Modified after Tsang and Tsang [1987].

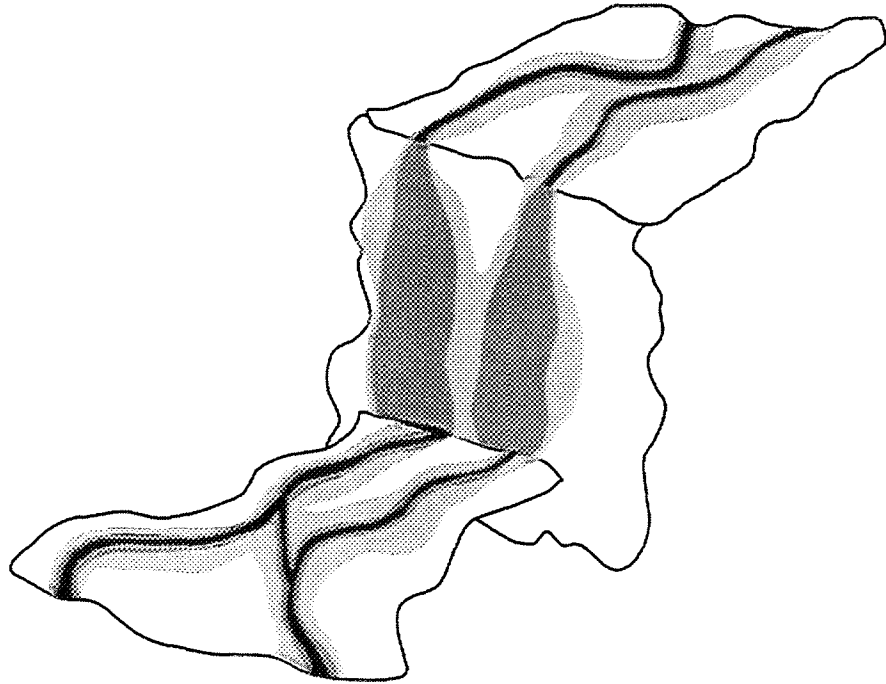


Figure 2.2 Conceptual description of flow paths through a set of fractures. Modified after Tsang and Tsang [1987].

Since the flow wetted surface is a function both of the properties of the rock (fracture geometry) and of the flow field within the rock it cannot strictly be considered to be an intrinsic material property, but is dependent on flow situations and boundary conditions [Olsson, 1995, Selroos and Cvetkovic, 1996]. However, in practice it is often treated as such, for example in transport models used in several safety assessments (Section 4).

2.1 Specific flow wetted surface

Many radionuclide transport models used for safety assessments of spent fuel repositories are based on the stream tube concept. A stream tube is an imaginary tube defined as a volume enclosed by a surface made up of a set of stream lines. The complex three-dimensional flow field is thus divided into a set of independent one-dimensional stream tubes. Each stream tube contains both water bearing fractures and rock matrix accessible to the radionuclides only by diffusion. The radionuclide transport in the stream tube is normally calculated using the advection-dispersion equation.

Since the rock volume encompassed by a stream tube will contain many channels, fractures or other flow paths, it is useful to employ the concept of specific flow wetted surface, eg by defining the flow wetted surface as the contact area between the flowing water fracture surfaces **per unit volume of flowing water**, here denoted a_w . This is practical in applications where the radionuclide velocity is linearly related to the water velocity.

For sorbing radionuclides it can be shown that the radionuclide velocity in the rock is in practice independent of the linear velocity of the water in the fractures [Neretnieks, 1987]. The nuclide velocity is then determined by the water flux (Darcy velocity). In this case it may be more convenient to use the flow wetted surface **per unit volume of rock**. This is denoted as a_r . The two ways of expressing flow wetted surface can be related by:

$$a_r = a_w \varepsilon_f \quad (1)$$

where ε_f is usually taken as the flow porosity. However, the relation is only approximate since the flow porosity takes only into account the part of the fracture with flowing water and not parts with stagnant water. Furthermore, the flow porosity is an averaged parameter found to be very sensitive to the size of the averaging volume. It is also a parameter that is difficult to measure accurately in the field.

2.2 Relation between flow wetted surface and water flux

A major problem in the definition of flow wetted surface is to properly describe the relation between the flow wetted surface and water flow rate. One alternative formulation for defining the efficiency of transfer between the water and the rock is to use the **ratio flow wetted surface to water flux**.

The ratio between flow wetted surface to water flux can be derived directly from assumptions on the characteristics of the flow paths within the rock. In the case of parallel channels with width W and length L , and with a flow rate in the channel Q , the ratio may be given as:

$$\frac{2WL}{Q} \quad (2)$$

This parametrization has been used in discrete models, such as the channelling model [Neretnieks, 1983] and the channel network model [Moreno and Neretnieks, 1993].

For a rock volume encompassed by a stream tube containing many flow paths, it is useful to use the concept of specific flow wetted surface, a_r , ie, all the flow wetted surface area per volume of rock in the stream tube. In this case the ratio of flow wetted surface to water flow rate can be defined as:

$$\frac{a_r L_{path}}{q} \quad (3)$$

where q is the water flux (Darcy velocity) and L_{path} is the length of the flow path. The higher this ratio is the larger is the retarding effect due to matrix diffusion and sorption. This type of parametrization has been used in the TVO-92 study (*transport resistance*) [Vieno et al, 1992] and in the SITE-94 study (*F-ratio*) [Andersson et al, 1995; SKI, 1996] as a way of defining the transport parameters for the radionuclide transport model, see Sections 4.3 and 4.4 below. In the

SITE-94 study the F-ratio was found to be much less sensitive to the size of the averaging volume than the flow wetted surface per volume of rock, a_v .

It should be noted that the local value of the ratio between the flow wetted surface and the water flux is important. Thus averaging a_v along the flow path independently of how q varies and averaging q along the flow path independently of how a_v varies, as is currently done in many advection-dispersion models, can lead to considerably different results compared to averaging of the ratio a_v/q . However, it is not presently possible to measure the ratio a_v/q locally. In some model concepts it is possible to assign local values to the ratio a_v/q , eg channel models, channel network models or fracture network models.

Although flow occurs only in part of the fracture, the zones with more or less stagnant water can be accessed by diffusion. Thus, also the rock matrix in contact with the stagnant water can be accessible for matrix diffusion and sorption. This has been used as an argument to question the traditional way of defining the flow wetted area [Olsson, 1995]. It is argued that the flow wetted surface is considerably larger than what could be deduced from the flow rate distribution. Also the accessible surface for matrix diffusion would tend to increase with time as radionuclides diffuse further into the stagnant water.

Surfaces of fractures are often rough and the fractures may also contain infillings. Thus, the actual surface area may be considerably larger than the geometrical area. However, the irregularities of the fractures usually have a very small volume and may therefore be of less importance for matrix diffusion and sorption at long time scales and for less sorbing radionuclides. Figure 2.3 illustrates the actual surface and the surface as "seen" by a radionuclide that has diffused some depth into the matrix.



Figure 2.3 Cross-section of a fracture with actual surface of fracture (solid line) and surface as seen by a radionuclide diffused some depth into the matrix (dashed line).

3 Methods for determination of flow wetted surface

Several methods have been proposed to assess the flow wetted surface. Some of these have been tried in practice while others need yet to be developed. In this chapter a brief overview of various proposed methods is made, including a short discussion on advantages and disadvantages of the methods.

3.1 Tracer migration experiments

The use of tracer migration experiments for addressing the issue of the flow wetted surface is apparently straightforward. However, tracer tests do not actually measure the flow wetted surface, instead a number is derived by fitting the test results to a model. A large number of tracer experiments have been performed in fractured media [Anderson, 1995]. The basic idea is to perform tests with sorbing and non-sorbing tracers and from the difference in travel time distribution draw conclusion about the effective retardation of the sorbing radionuclide. The tracer tests can be performed in such a way that they more or less simulate the expected conditions in a repository situation. However, there are several practical and theoretical problems involved in doing this.

- in most tracer experiments only a limited amount of the tracer is recovered at the collection point
- it is difficult to find sorbing tracers that have short enough residence times in the rock to allow for experiments over sufficiently long distances within reasonable time
- the evaluation and extrapolation of the results are not straightforward

The theoretical problem mostly concerns how tracer experiments should be evaluated. A traditional way of doing this is to take the ratio between the sorbing tracer travel time and the non-sorbing tracer travel time to derive an effective retardation factor characteristic of the rock. However, it is argued [Neretnieks, 1995] that a retardation factor derived in such a way only relates to the specific test situation and has no predictive capability. Thus, it could not be used to predict sorbing tracer travel times for other environments, longer travel distances or even for other flow situations at the same location. The reason being that the travel times for non-sorbing tracers are determined by the flow porosity, while this parameter is of negligible importance for sorbing tracers. Instead, the sorbing tracer travel time depends on the flow wetted surface, and the diffusion and sorption properties of the rock. These effects have been demonstrated using various types of simulation models [Moreno et al, 1995].

On the other hand, it is also argued that tracer experiments with non-sorbing tracers and water residence times derived from such experiments provide necessary information for predicting the transport of sorbing radionuclides [Cvetkovic, 1995]. The basic theory is that there are two competing mechanisms for sorbing tracer movement in fractured rock: solute advection by a heterogeneous water flow field, and solute mass transfer with immobile water (eg matrix diffusion) and the solid rock (eg sorption). The reactions along a stream tube are characterized by a function $\gamma(t, \tau)$, where t is time and τ is the water residence time. The residence time distribution of the sorbing tracer can be obtained by integrating γ with the residence time distribution of the water (RTD). The function γ takes complex forms that can be obtained either analytically or numerically. The function can be divided into parts, one describing the physical-chemical effects and another describing the influence of flow path geometry. In a further study [Selroos and Cvetkovic, 1996] an attempt has been made to find correlations between the residence time distribution of water and the function describing the geometrical effects by simulations of a simplified channel in a fracture with varying aperture and width.

Tracer migration experiments have been used to make estimates of the flow wetted surface, for example in the Stripa 3D-experiment [Abelin et al, 1987]. The flow wetted surface was determined by comparing the experimental recovery with the recovery predicted by model calculations assuming that the non-recovered tracer was taken up into the rock matrix by matrix diffusion. The model predictions used data on matrix porosity and diffusivity from laboratory diffusion measurements. The flow wetted surface per unit volume of rock was estimated to be between 0.2 and 2 m²/m³, with indication of values possibly as high as 20 m²/m³.

Tracer experiments in a fracture zone have been performed in the Stripa SCV study [Birgersson et al, 1992]. Here attempts were made to estimate the flow porosity and flow wetted surface by fitting the residence time distributions of tracers with dye and complexed metals to an advection-dispersion model. This also required estimates of the mean fracture aperture. A fracture aperture of 0.3 mm yielded estimates of the flow wetted surface per volume of rock between 5 and 24 m²/m³. The flow wetted surface was also estimated by interpreting the flow and transport data using the channel network model, also using channel widths from the channelling experiment [Abelin et al, 1990]. This yielded a much lower value, 0.1 m²/m³. The large difference in the prediction is suggested to be caused by uncertainties in the porosity estimates. In connection with investigations of the flow distribution in a fracture zone at the Stripa mine using tracer injection and bore hole radar the flow wetted surface was estimated to be 1.8 m²/m³ rock [Andersson et al, 1989].

Evaluations of the flow wetted surface has been made from a tracer experiment in a low angle major fracture zone at the Finnsjö site [Gustafsson and Nordqvist, 1993]. The flow wetted surface was estimated from the number of fractures within the fracture zone, the fraction of preferential flow paths and the width of the fracture zone. The flow wetted surface per volume of rock was estimated to be between 1 and 92 m²/m³, assuming no reduction due to preferential flow

paths. The flow wetted area per volume of flowing water was estimated based on fracture apertures to be between 1180 - 8700 m²/m³ of water.

Within the ongoing Tracer Retention Understanding Experiments (TRUE) at Äspö Hard Rock Laboratory [Bäckblom and Olsson, 1994] a number of experiments giving direct or indirect information on the flow wetted surface will be performed. In the First TRUE stage [Winberg, 1994] a number of small scale tracer tests will be performed with conservative tracers: dilution tests, radially converging tests, dipole tests and radially diverging tests. The emphasis on these tests is on the advective and dispersive features of the transport, focussing on the effect of heterogeneity on solute travel time distributions. In the Second TRUE stage tracer tests on a block scale (≈ 50 m) are planned with the objective to test and evaluate scaling relationships and to test model predictions for tracer transport in a network of fractures.

3.2 Tunnel observations

One source of information for determining the flow wetted surface has been observations of the width of water bearing channels in tunnels and drifts. In a tunnel or drift large rock surfaces can easily be surveyed. From observations in a 4.5 km long full-face drilled at Kymmen in western Sweden it was found that 99.7% of the channels were less than 0.1 meter wide [Palmqvist and Lindström, 1991]. Based on the observed channel frequencies and a channel width of 0.1 m the flow wetted area per volume of rock was estimated to 0.006 m²/m³ for the rock mass and 0.03 m²/m³ for the fracture zones [Moreno and Neretnieks, 1993]. In observations of the tunnels and drifts of the Swedish repository for intermediate and low level waste (SFR) most channels were found to have a width in the order of a few decimeters, but a large number of point spots occurring at fracture intersections were also observed [Neretnieks, 1987]. With the assumption that the channel widths are 0.1 m, the flow wetted surface per volume of rock was estimated to be 0.02 m²/m³ [Moreno and Neretnieks, 1993]. A similar evaluation of observations at the Stripa mine gives an estimate of a , of 0.2 m²/m³. In the channeling experiment performed at Stripa the channel widths were found to be in the order of decimeters or less [Abelin et al, 1990].

The validity of such data has been questioned with the argument that the flow at the walls of a tunnel is severely disturbed by the changes in rock stress that closes or opens fractures, excavation damages and due to the intrusion of air into fractures [Olsson, 1995].

Indications of the importance of these effects were obtained from the Stripa SCV site. Six parallel bore holes, each with a length of 100 m, positioned in a circular shape were drilled and the inflow through a part where the holes intersected a fracture zone was measured, first with the boreholes drained one at a time, and secondly with all bore holes drained. Afterwards, the rock within the perimeter of the boreholes was excavated and the inflow to the excavated drift was measured. The measurements showed that the inflow decreased almost an order of magnitude after the excavation of the drift. Furthermore, a considerable

redistribution of the inflow locations was noted. This has been taken as an example that the concept of channelling can be drastically misled by tunnel observations [Olsson, 1995].

Despite the known difficulties it is still argued that examinations of tunnel walls give some indication of the distribution of flow within the rock. However, the use of observations for quantitative estimates may be limited.

3.3 Borehole information

The estimation of the flow wetted surface from borehole information is based on the concept that the frequency of water bearing fractures intersecting a borehole is a function of the width and the length of the flow channels. In the case the bore hole diameter is small compared to the width of the channel, the flow wetted surface can directly be derived from the average spacing between the water conducting fractures [Moreno and Neretnieks, 1993; Gylling et al, 1994]. The method was originally developed to provide data on channel lengths for the channel network model when channel widths can be evaluated independently. The method is based on the assumptions that the apertures of the channels are much smaller than the other dimensions of the channels, the channels are small in relation to the average distance between them and that the orientations of the channels are random. When the method is used to determine the flow wetted area no further assumptions are needed about the widths or geometric structure of the channels, as long as the widths are much larger than the bore hole diameter.

To obtain the necessary information a bore hole has to be measured using a very small packer spacing. A problem is involved in determining what is a conductive fracture. In practice, the measurement limit in the packer test will determine if a section is conductive or not. One method to estimate also the number of low conducting channels is to assume a log-normal distribution of the fracture flow rate. Thus, the distribution of fractures with non-measurable flow is extrapolated from the known distribution of fractures with measured flow. If the extrapolation is valid, this could be a way of assessing the area where radionuclides could access the matrix although the flow rate is very low.

The method has been applied to bore hole data from Stripa [Geier et al, 1990], based on the conductive fracture frequency, the bore hole diameter and an assumed fracture width of 0.1 m the flow wetted surface per volume of rock was estimated to $0.4 \text{ m}^2/\text{m}^3$ [Moreno and Neretnieks, 1993].

An advantage with the method of deriving data from bore hole information is that it will provide information both on the flow wetted surface of the water bearing features and their water flow rate. This information is obtained on a local scale suited for a model such as the channel network model. It cannot be directly applied to flow paths from a repository to the geosphere, since it does not give information on how the channels connect. However, it can also provide valuable information for other discrete models such as fracture network models.

The present model assumes random orientation of the water bearing channels, whereas fractures often have preferential orientation. However, an extension of the model to also consider fracture and bore hole orientation seems feasible.

A debated question is to what degree flow rate distributions to bore holes, under boundary conditions that may be different from those representative for transport from a repository, are a good measure for the flow wetted surface [Olsson, 1995].

3.4 Fracture characterization

The flow wetted surface is strongly related to the physical characteristics of the fracture. Fracture aperture distributions are vital input data for theoretical models of flow and transport in fractures. Several methods have been used and are being developed for visualizing fractures in rock samples [Degueldre et al, 1996]. These include physical transmission or tomographic methods such as Nuclear Magnetic Resonance Imaging (NMR), Neutron radiography and Positron Emission Tomography (PET) and methods where a polymer resin is injected into the fractures which are subsequent cut and measured.

The resolution of the physical methods is presently limited to a few hundred to a thousand μm and may not be suitable for accurate aperture measurements. However, with suitable fluids the flow pattern can be investigated in ongoing experiments, a method used in petroleum research [Chen et al, 1996]. The measurements have so far been used only on samples with dimensions of a few centimeters.

Within the ongoing Tracer Retention Understanding Experiments (TRUE) at Äspö Hard Rock Laboratory a resin injection experiment is planned with the objective to obtain a qualitative picture of the flow path geometry and provide data for estimating fracture apertures [Birgersson and Lindbom, 1995; Birgersson et al, 1995]. An epoxy resin will be injected in a fracture that has been characterized by hydraulic test and tracer tests with sorbing and non-sorbing tracers. The investigated part of the fracture plane is located quite far away from the drift in order to maintain an undisturbed mechanical situation. The fracture will be sampled using large diameter cored boreholes. The injected resin will be analyzed to provide data on the pore space distribution in undisturbed fractures. Such data can for example be used by stochastic fracture models and indirectly provide information on the flow wetted surface.

3.5 Geochemical effects

3.5.1 Red coloring of rock

Fracture surfaces are often found to have patches with distinct red coloring. It has been proposed [Olsson, 1995] that investigation of the extent of red coloring along fracture traces could be a means of determining the distribution of flow within the fracture plane and thus give a measure of the contact area between the flowing water and the rock. The origin of the coloring in Swedish granites from Äspö and Stripa as well as of weathered rinds at a glacial polished rock surface of Bohus granite has been studied [Eliasson, 1993]. It was found that the red-colouring of the Äspö granite was due to presence of fine-grained Fe-oxyhydroxides and hydroxides most likely as a result of hydrothermal alterations, also causing distinct changes in mineralogy and porosity. The red coloring of the Stripa granite was explained by oxidation and reprecipitation of iron as hematite and to less extent as Fe-oxyhydroxide during slightly oxidizing conditions in a basically isochemical system. For the Bohus granite weathering and precipitation of Fe-oxyhydroxides and hydroxides as a result of the last 12 000 years at atmospheric conditions is responsible for the coloration of the rock.

A major problem with using red coloring as a means of assessing the flow wetted surface is that very little is known about the flow conditions during the period when the geochemical alterations were active. As the flow wetted surface is dependent on the flow situation and boundary condition, any extrapolation to present day or future situations are highly uncertain. This is especially the case when red coloring is caused by hydrothermal alterations which occur at temperatures of several hundred degrees.

The more recent red coloring due to infiltrating oxidizing water may also be affected by the often very long time scales in the oxidation reactions. Thus, the extent of the red coloring is not only a function of the contact area between water and rock, but also on the movement of oxidation fronts. This makes interpretation of the results difficult. Despite the difficulties to make quantitative estimates from studies of red coloring of rock, they may prove valuable for the understanding of surface interactions and how these change in the long-term perspective.

3.5.2 Radon concentration in groundwater

Radon measurements have been used to assess the fracture surface area of geothermal reservoirs [Nicol and Robinson, 1990]. The Rn-222 flux measured from plane rock surfaces was used in conjunction with a simple hydrological model to calculate the Rn-222 content in the return fluid of the geothermal system. By matching the calculated and measured contents the extent of the heat transfer surface was estimated [Andrews et al, 1986]. However, such estimates have been found to give 25-45 times larger estimates of the surface area than the effective heat transfer surface area observed [Hussain, 1991]. The lower

effective heat transfer surface area was attributed to the clustering of fractures within the range affected by heat transport.

The emanation of radon from uranium bearing rock has been tested as a method to estimate the flow wetted surface [Glynn and Voss, 1996]. The estimate is based on the assumption that the Rn-222 content in groundwater is related to uranium content in the rock and the flow wetted surface. From Äspö data on the uranium content in the rock and the radon content in the water a flow wetted surface of $3100 \text{ m}^2/\text{m}^3$ water was derived. Using the low end flow porosities from the LPT2 test (10^{-4} - 10^{-2}), that is 10^{-4} - 10^{-3} , a range for the flow wetted surface per volume of rock between 0.31 - $3.1 \text{ m}^2/\text{m}^3$ was obtained.

The method can be expected to be more applicable for estimating the flow wetted surface for radionuclide transport than for estimating effective heat transfer surface area as the range affected by transport should be more similar. However, the method requires a number of assumptions concerning the release and transport of radon which adds to the uncertainty in the results. Possibly the method could be used at sites with well characterized uranium content in the rock to investigate large scale variations in the flow wetted surface.

3.6 Theoretical modelling

Discrete fracture network models have been used as a means for estimating the flow wetted surface. In these models a network of fractures is generated stochastically in a three-dimensional space. The fractures are modelled as simple geometrical structures such as discs [Andersson and Dverstorp, 1987; Cacas et al, 1990; Dershowitz et al, 1991] or rectangles [Herbert, 1988]. The distributions for their random size and orientation are derived from statistics from fracture mapping. Various statistical procedures have been developed for positioning of the fractures. In some models large scale features such as fractures zones or known fractures can be modelled deterministically [Geier, 1996]. Transmissivities of the fractures are also given stochastically, but often calibrated to correspond to the large scale hydraulic conductivity.

Transport within the individual flow paths is often modelled by using a finite number of “particles” representing the radionuclide. The advection is described by letting the particles follow the flowing water. The dispersion may be described by applying a random walk technique. However, the dispersion within the individual flow paths is often found to be of minor importance compared to the dispersion caused by variations in flow between flow paths, and is therefore treated in a simplified way or even neglected. Retardation effects due to surface sorption may easily be incorporated in such models, while the modelling of retardation effects due to matrix diffusion and sorption in most applications requires extensive computer resources.

One method to use discrete fracture network models to assess the flow wetted surface is to perform “synthetic” tracer experiments. Simulations are performed both with a sorbing and a non-sorbing tracer within the same discrete fracture

network. A one-dimensional advection-dispersion equation is then fitted to the mass release curves obtained from the tracer experiments to obtain a value for the effective flow wetted surface. This methodology has been used within the Project-90 [Dverstorp, 1991] and SITE-94 projects. An alternative method is to estimate the flow wetted surface by integrating the flow wetted surfaces of the individual fractures making up the flow paths. The selection of flow paths can be made from the particle tracking [Geier, 1996] or by first determining the dominating flow paths, eg by directed search [LaPointe et al, 1995].

Estimating the flow wetted surface from discrete fracture network modelling, requires some assumptions concerning the flow wetted surface within the individual fractures constituting the flow path. Generally, the transport flow paths within the fractures are estimated as cylindrical tubes or plane parallel fractures with dimensions adjusted to the transmissivity of the fracture [Dverstorp, 1991]. The cylindrical tube gives the lowest flow wetted surface theoretically possible, while a plane parallel fracture with all surfaces accessible gives a value in the high end range. Higher values than for the plane parallel fracture can be obtained if the fracture surfaces are highly irregular or if fracture infillings are considered.

Within the SITE-94 study a sensitivity analysis was performed on flow wetted surface parameter using a discrete fracture model [Nordqvist et al, 1995, 1996]. A set of fractures were generated stochastically within a three-dimensional space, where each fracture had transport properties determined assuming variable apertures within the fracture. The aperture distribution was assumed to be lognormal. As it is a resource demanding calculation to solve the flow and solute transport in a collection of variable aperture fractures simultaneously, a two-step approach was used. In the first step the flow and solute transport within individual fractures was solved using the methodology of Moreno et al [1988], i.e. the fracture plane is discretized into a square grid, where the aperture of each grid block is assigned using geostatistics. The solute transport within a number of such grids is solved to generate a library of fracture transmissivities and residence time distributions. In the next step each fracture in the three-dimensional network was randomly associated with a library fracture. The transmissivities of the library fractures were adjusted to correspond to that of the network fractures. Once the flow in the fracture network is obtained, the residence time of a particle is determined by consecutive sampling of residence times from the distributions of the associated library fractures. A breakthrough curve for solute transport in the network is obtained by calculating the transport times for a large number of particles.

The estimated median flow wetted surface varied between 0.2 and 5 m²/m³ rock. The estimate was found to be relatively insensitive to the model parameters that were varied with the exception of the variance in the aperture. For the low aperture variance (standard deviation in log b, $\sigma=0.43$) a flow wetted surface in a narrow range of 3-4 m²/m³ rock was found, while the case with a high aperture variance (standard deviation in log b, $\sigma=1.17$) gave slightly lower values, but with a larger range, 0.2-2 m²/m³ rock.

The method using discrete fracture network modelling does not give independent estimates of the flow wetted surface in the real rock, since the flow wetted surface for the individual fracture has to be assessed by other means. In the fracture network model used for the SITE-94 study [Nordqvist et al, 1995], where each fracture was modelled separately, the flow wetted surface was found to be very dependent on the value used for the variance of fracture apertures. However, the approach gives valuable insights on the implications of variations of the effective flow wetted surface area for different flow paths as it directly connects the flow wetted surface with the flow rate in the flow path. Thus, it can be a means of identifying the possibility of having fast flow paths in the rock with very low specific surface area. Simulations performed with sorbing tracers [Nordqvist et al, 1996] show that both mean retardation and the shape of the breakthrough curve depend strongly on the degree of heterogeneity in the flow paths. For a high variance of fracture apertures the retardation due to linear surface sorption was found to be significantly smaller than the retardation derived by using the mean aperture. These results demonstrate that the application of a retardation factor may be misleading in heterogeneous systems.

3.7 Heat transport and storage in rock

Study of heat storage in rock is another area where the contact area between the flowing water and the rock is an essential parameter. In the characterization of the geothermal reservoir, experimental and theoretical studies are used to quantify the effective heat exchange area. The heat in the rock is transferred from the rock matrix mainly by conduction to the fractures where it is transferred mainly by convection. Thus, the situation is analogous to the case of radionuclide transport in rock, with the differences that the transfer of heat instead of mass is studied. The effective heat exchange area should be analogous to the flow wetted surface studied for radionuclide transport. However, many studies on heat storage are made for rock types different from those considered for deep disposal. Furthermore, the rock used for heat storage is often affected by hydraulic stimulation (high pressure injection of water or other fluids) to increase the permeability of the reservoir.

The main effort is usually to define the total effective heat exchange area for the reservoir using models with many similarities to the advection-matrix diffusion models used for radionuclide transport. However, as the total volume of the reservoir is usually not well known, these total areas cannot always be transferred into specific areas per volume of rock or per volume of flowing water.

In a study of the heat extraction from the geothermal reservoir in hot crystalline rock in Wales [Nicol and Robinson, 1990] theoretical models were compared with tracer experiments and the measured heat extraction. In the reservoir three wells, more than 2000 meter deep, have been drilled. The permeability of the reservoir was enhanced by hydraulic stimulation. Investigations concluded that the permeability increase was mainly due to the increased aperture of existing joints, not the formation of new joints. An average water flow of about 20 kg/s

was injected in one well, whereof 75% have been withdrawn from the other. The temperature of the outlet water has been between 55 and 80°C.

The study found that although the reservoir was highly fractured (average horizontal spacing 1-2 meters) it did not behave like a porous media. Instead the flow was concentrated to a limited number of zones with a horizontal spacing of 10-25 meters. Furthermore, it was found from the thermal analysis that a few independent flow paths could be identified, one with a little more than 10% of the flow and with a significantly lower effective surface area. However, no zone for entry of the heated water has been identified as containing this short circuit. In addition tracer test results were used to further constrain the choice of parameters. The effective heat exchange area was found to be between 0.05 and 0.08 m²/m³ rock.

Studies of analogues between radionuclide transport and the thermal behavior of rock seem to be a promising approach for increasing the understanding of interactions between flowing water and solids in fissured rock. In principal, the heat transport is used as a reactive tracer which is used in conjunction with the results of tests with non-reactive tracers. Temperature measurements can easily be made with high precision at short intervals. The results of such tests are on a form very similar to the F-ratio used in the SITE-94 study. However, heat conduction is several orders of magnitude faster than molecular diffusion, which has advantages as well as disadvantages. Thus, the scaling between diffusion and flow part will be different from heat transport and radionuclide transport. Also heat will diffuse much further into the rock than dissolved tracers, which means that a larger part of the rock matrix will take part in the "sorption" in the case of heat transport compared to the case with radionuclide transport. Thus various geometrical aspects may be different, eg the effect of neighbouring fracture may not be neglected as often is the case for radionuclide transport where the matrix sometimes is approximated as a semi-infinite medium.

In a pilot dipole experiment with heat transport has been performed by Nagra at Grimsel salt and heat was injected in a fracture system and monitored at the extraction point [Marschall and Vomvoris, 1995; Liedtke et al, 1994]. The method was judged to be suitable for moderate and high permeability rock for experiments performed over distances of 10 to 20 meters.

3.8 Discussion

The various experimental methods used to determine the flow wetted surface can be divided into three types:

- methods based on estimation of flow path dimensions, eg channel widths from tunnel or bore hole observations or fracture aperture from fracture measurements.
- methods based on evaluation of the effect of interactions at the flow wetted surface, eg sorption of tracers, release of radon or exchange of heat.

- methods based on evaluation of geological evidence of surface interactions, eg geochemical alterations giving red coloring.

Various theoretical models are used in combination and in addition to these experimental methods to evaluate the results and attempt to extrapolate to longer distances.

Data from observations of tunnels and bore holes provide an estimate of the flow wetted surface per volume of rock, a_r . Thus, the estimates can be used directly for predicting the transport of sorbing species without the need of accurate values of the flow porosity. These methods have been tried and found to give reasonable predictions. However, the method does not directly measure the interaction area, as low flow rate flow paths and stagnant zones cannot be measured, instead these have to be estimated by extrapolations. There are also problems associated with making observations without disturbing the flow in the rock.

Data on fracture apertures provides an estimate of the flow wetted surface per volume of water, a_w . In order to convert this into an a_r , an estimate of the flow porosity is needed. Fracture network simulations have shown that estimates based on average apertures may significantly underestimate the retardation in systems with a high variability of fracture apertures. However, data on fracture aperture distributions will provide valuable input data for theoretical models (eg fracture models with a stochastically varying fracture aperture) that can be used for estimates of the flow wetted surface.

The methods based on the evaluation of interaction effects can provide estimates of the actual surface of interaction between fracture and matrix. However, the methods are associated with several practical and theoretical problems. The migration of tracers is the method most similar to the problem of transport of radionuclides in the far-field, but in practice it is difficult to perform experiments with sorbing radionuclides over long distances within reasonable time. Most of the tracer tests have so far been performed with non-sorbing tracers. Therefore analogous systems such as transport of heat in fractured rock seem to be worthwhile investigating, possibly in combination with tracer tests.

Evaluation of geological evidence of surface interactions has so far not been extensively used. It is therefore not possible to judge how useful the method may prove to be. In general, studies of natural analogues tend to give more qualitative information concerning the presence and magnitude of various processes than quantitative data.

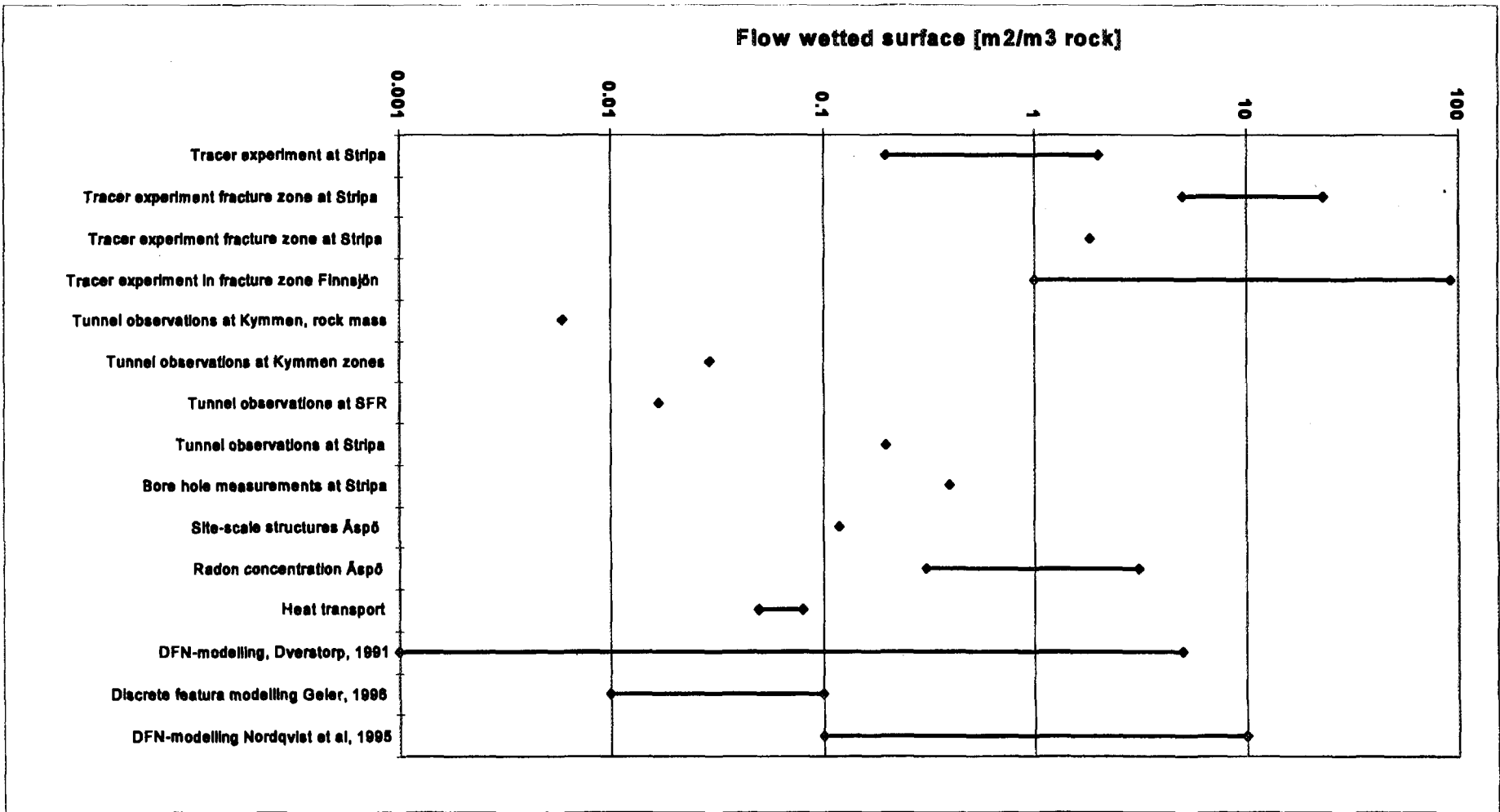
In Table 3.1 and Figure 3.1 a summary is given of estimates of the flow wetted surface made by various methods. There is a large variability in the values depending both on the type of method used and on the characteristics of the rock. The result of tracer tests and observations of fractures span about 3 orders of magnitude for the rock mass ($0.006-3 \text{ m}^2/\text{m}^3 \text{ rock}$). The variability in the values for fracture zones is 3.5 orders of magnitude ($0.03 - 92 \text{ m}^2/\text{m}^3 \text{ rock}$). Although the data is limited, there is a tendency that estimates based on observations in

tunnels and measurements in bore holes give lower values than tracer tests and measurements of radon concentration.

Table 3.1 Summary of estimates of the flow wetted surface.

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 tests at Stripa [Abelin et al., 1987]	0.2 - 2 (possibly up to 20)	
Tracer tests in fracture zone Stripa [Birgersson et al 1992]	5 - 23	
Tracer injection and borehole radar in fracture zone Stripa [Andersson et al, 1989]	1.8	
Tracer test in fracture zone Finnsjön [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 Äspö [Voss et al, 1996]	0.12	
Uranium content and radon concentration Äspö [Glynn and Voss, 1995]	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, 1995]	0.1 - 10	

Figure 3.1 Summary of estimates for flow wetted surface.



4 Application of flow wetted surface in safety assessments

This section gives an overview of how the flow wetted surface has been treated in various safety assessments from 1983 to 1996. A short review is made of the derivation of data, the parametrization in the models, the values used in the modelling and the main results.

4.1 KBS-3

In the KBS-3 study radionuclide transport was modelled in a single one-dimensional flow path from the repository to a nearby fracture zone. A constant water flow rate and an average or shortest length of the migration path was used. The modelled domain consisted of a straight tube containing both the water bearing fractures and the blocks of rock. The tube had a constant water velocity and thus a constant cross-sectional area. The water flux was assumed to be $10^{-4} \text{ m}^3/(\text{m}^2, \text{a})$. A one-dimensional advection-dispersion model including the effects of matrix diffusion and sorption was used.

The flow wetted surface was based on bore hole observations on the frequency of water bearing fractures. At levels below 300 meters a hydraulic fracture frequency of $0.2 - 0.3 \text{ m}^{-1}$ was found at the Finnsjön site and $0.1 - 0.2 \text{ m}^{-1}$ at the Sternö site. For the safety analysis a hydraulic fracture frequency of 0.2 m^{-1} was used, i.e. an average spacing between water bearing fractures of 5 meters. As no reduction of the available area due to channelling was considered, this gives a flow wetted surface per volume of rock, a_r , of $0.4 \text{ m}^2/\text{m}^3$. With the flow porosity of 0.0001 (corresponding to a mean fracture aperture of 0.5 mm), a flow wetted surface per volume of flowing water, a_w , of $4000 \text{ m}^2/\text{m}^3$ was obtained.

4.2 SKB 91

In SKB 91, a set of streamlines from different parts of the repository to the biosphere were calculated by particle tracking in the hydrological model (HYDRASTAR) [Norman, 1992]. Each streamline represented a streamtube with a cross-section area of about $10\,000 \text{ m}^2$ at repository level. The total groundwater travel time for each streamtube was used by the radionuclide transport model (FARF31) [Norman and Kjellbert, 1990] to calculate the radionuclide transport along the stream tube, assuming a constant flow porosity throughout the rock. The transport parameters in FARF31 (Peclet number, flow wetted surface, matrix diffusivity, sorption properties) are required to be

constant along the stream tube. This implies that averaged effective parameters must be used when applying FARF31 to a stream tube with varying properties.

For the reference scenario a flow wetted surface, a_r , of $0.1 \text{ m}^2/\text{m}^3$ rock was selected [Elert et al, 1992]. This value was taken as a central value in a possible range from 0.01 to $0.5 \text{ m}^2/\text{m}^3$. The range was derived from results from tracer experiments in Stripa [Abelin et al, 1987], observations of channel widths in tunnels and drifts [Neretnieks, 1987; Palmqvist and Lindström, 1991; Abelin et al, 1990].

4.3 Project-90

The problem of assessing the flow wetted surface (referred to as “the specific surface area between the rock and the flowing water” in their reports) was addressed in Project-90. A review was made of various experiments that sought to quantify the flow wetted surface. Furthermore, analysis was made using a discrete fracture network model [Dverstorp, 1991]. The flow wetted surface was estimated by first calculating the transport of a non-sorbing tracer through the simulated discrete fracture network and then simulating the transport of a sorbing tracer in the same network. A one-dimensional advection-dispersion model is then fitted to the breakthrough curves obtained from the numerical experiments.

The discrete network parameters were calibrated to the Stripa 3D experiment, studying the effect of three types of local fracture geometries: circular tubes, 0.2 meter wide channels and flow in the entire fracture plane. The fracture apertures and tube radius were adjusted to give equivalent fracture transmissivities. The results showed that if the flow is confined to circular tubes the flow wetted area, a_r , may be as low as $0.001 \text{ m}^2/\text{m}^3$ rock and in the case of flow in the entire fracture plane as high as $5 \text{ m}^2/\text{m}^3$ rock. It was argued that both values were unrealistic extremes; a network of circular tubes would not produce flow porosities consistent with observed values and studies of variable aperture single fractures indicate that the flow is confined to a few channels in the fracture plane. A flow wetted surface per volume of rock of $0.01 \text{ m}^2/\text{m}^3$ was chosen as a pessimistic, but not totally unrealistic reference value. In the parameter variations a value of $1 \text{ m}^2/\text{m}^3$ rock was used, described as an “optimistic value”.

The performed parameter variations showed that the flow wetted surface was the parameter that had the greatest effect on the delay of sorbed radionuclides.

It was recommended that field experiments should be performed specifically to try to measure the flow wetted surface, with special focus on whether rock with a low flow wetted surface may extend over large domains, and if such domains are correlated with high flow channels.

4.4 TVO-92

In the Finnish TVO-92 safety analysis of spent fuel disposal [Vieno et al, 1992] the effect of matrix diffusion and the contact surface between the rock and the flowing water have been analyzed.

The radionuclide transport in the geosphere is modelled in a single flow path going from the repository through the rock matrix into a fracture zone. Several alternative flow paths were evaluated, including transport through the disturbed zone around the repository. The flow path giving the least transport resistance was chosen for the reference scenario.

The migration is assumed to take place in channels in the rock. In TVO-92 a somewhat different terminology is used. The channels are characterized by a total channel width per rock area, (here denoted W' not to confuse with channel width W), and the total length of the flow path, L . The flow wetted surface defined as "the rock surface in direct contact with groundwater flowing in the channels" is given by $W'L$. This entity does not correspond to the specific flow wetted area per rock volume, a_r , which would be given by $2W'$. In the comparison between the alternative flow paths a "total transport resistance" defined as $W'L/q$ is used, where q is the groundwater flux (Darcy velocity). The parameter W' has been estimated based on assumptions about fracture spacing and the percentage of total surface area covered by channels ($W'L/q$ of the TVO-92 report and the F-ratio of the SITE-94 report are related by $W'L/q = \frac{1}{2}$ F-ratio). In Table 4.1 data related to different parts of the rock are given.

Table 4.1 TVO-92 data on trace length of fractures per unit area.

Type of rock	Darcy velocity [l/m ² ,a]	W' [m/m ²]	W'/q [a/m ²]
Intact rock	0.1	0.02	200
Intact rock, high hydraulic conductivity	1	0.04	40
Disturbed rock zone	10	0.25	25
Disturbed rock zone, high hydraulic conductivity	100	1	10
Zone III ($T= 10^{-7}$ m ² /s)	10	0.6	60
Zone II ($T= 10^{-6}$ m ² /s)	50	0.8	16
Zone I ($T= 10^{-5}$ m ² /s)	150	1	7

The total transport resistance of the various alternative flow paths from the repository to the biosphere range from $1 \cdot 10^4$ - $7.2 \cdot 10^4$ a/m for typical values of water flow rates. For a more pessimistic case with higher flow rates, the total transport resistance range from $2.2 \cdot 10^3$ to $1.9 \cdot 10^4$ a/m. A value of 10^4 a/m was

chosen for the reference scenario. In the sensitivity analysis a “short-circuit” case was analyzed with a $W'L/q$ of $2 \cdot 10^3$ a/m.

The actual migration codes used in the TVO-92 study did not use the parameter total transport resistance, $W'L/q$. Instead, the code parameters: length of flow path, groundwater velocity and fracture aperture, were assigned in such a way that corresponding case was achieved.

The maximum dose rate was one order of magnitude higher in the “short-circuit” scenario ($W'L/q = 2 \cdot 10^3$ a/m) compared to the reference scenario ($W'L/q = 10^4$ a/m). This is due to increased release rates of radionuclides with a relatively short half-life and moderate to strong sorption in the rock (Ra-226, Pu-239, Pu-240, Am-243).

A simple analysis was also made of the effect of stagnant pools on retardation. The analysis considered only the effect of the stagnant water phase, neglecting the increase in accessible rock surface for matrix diffusion and sorption. The results indicated that stagnant pools may have a more significant effect than matrix diffusion for weakly sorbing radionuclides. However, this effect was not considered for the safety analysis.

4.5 Kristallin-I

The project Kristallin-I conducted by NAGRA [NAGRA, 1994], investigated the possible disposal of high-level waste in the crystalline basement of Northern Switzerland. The project was based on the previous Project Gewähr [NAGRA, 1985], using the same but improved tools and databases.

The groundwater flow is assumed to take place in a network of discrete small water-conducting features. These features have been divided into three classes: cataclastic zones, jointed zones and fractured aplite/pegmatite dykes and aplitic gneisses. Each of these three types consists of sub-parallel, partially infilled fractures. For the far-field nuclide transport modelling performed there are no differences made between the cataclastic zones and the jointed zones.

In the far-field nuclide transport modelling the water conducting fractures are modelled as a single representative parallel-walled conduit or tubular conduit. The model was a 1D advective transport model including longitudinal dispersion (transverse dispersion was neglected), matrix diffusion, sorption and colloid enhanced transport. The siting of the repository is considered when assigning the length of the flow path. This is defined as the minimum distance from any part of the repository tunnel to either a major water conducting fault or the lower boundary of the higher-permeability domain.

Hydrogeological modelling and bore hole data provide data for the flow rate, path length and spatial density of water conducting features. Hydrochemical data provide data on colloid concentration and sorption. Geological data is used to determine the geometry and mineralogy of the water-conducting features.

A similar geometrical description is used for the internal structure of all three types of water conducting features in Kristallin-I. The density of water conducting fractures, γ [m^{-1}], is defined by the total trace length of features intersected by a plane. Each feature has a width of $2W$ [m] and consists of a set of fractures with a separation of $2y_3$ [m] and aperture $2y_1$ [m]. The total trace length of fractures per unit trace length of water conducting features is therefore equal to W/y_3 . Each fracture contains a set of channels, each with a width of $2x_1$. The channels are separated by a distance $2x_2$ in the fracture plane. Thus, the total trace length of channels per unit length of fracture is given by x_1/x_2 .

The flow porosity will be defined by:

$$\varepsilon_f = 2W\gamma \frac{x_1 y_1}{x_2 y_3} \quad (4)$$

The flow-wetted surface per volume of rock (in NAGRA [1994] denoted H) will be given by:

$$a_r = W\gamma \frac{x_1}{x_2 y_3} \quad (5)$$

and the flow wetted surface per volume of water will be defined by:

$$a_w = \frac{1}{2y_1} \quad (6)$$

The flow wetted surface per volume of rock varies between $0.0024 \text{ m}^2/\text{m}^3$ in the broad widely spaced channels in the western reference area to $0.17 \text{ m}^2/\text{m}^3$ in the fractured aplite/pegmatite dykes and aplitic gneisses in the eastern reference area. The flow wetted surface per volume of water was set to $1000 \text{ m}^2/\text{m}^3$ for all cases.

Through a series of simplifications, NAGRA arrived at 6 different geometries to analyze. The geometries differ in type of conduit (planar or tubular), extent of matrix diffusion (limited or unlimited) and type of water bearing fracture (cataclastic zones/jointed zones or fractured aplite/pegmatite dykes and aplitic gneisses). The geometry found to give the lowest retention in the geosphere was found to be case with widely-spaced channels in cataclastic zones/jointed zones with limited matrix diffusion.

4.6 SITE-94

SITE-94 is a repository performance assessment research project conducted by the Swedish Nuclear Power Inspectorate [SKI, 1996]. One of the main objectives was to develop a methodology for analyzing and propagating site specific data in a performance assessment. Within the project, the response of radionuclide release and transport models to potential uncertainties of both the engineered barriers and the geologic medium is explored. The purpose is to determine relative importance of different uncertainties and to provide insight into the

necessary precision for predictions of repository performance. The site evaluation was performed with real site characterization data from Äspö Hard Rock Laboratory.

The site scale hydrology was modelled using several different models:

- Simple evaluation using one-dimensional modelling [Dverstorp et al., 1996]
- Discrete feature modelling (3D) [Geier, 1996]
- Stochastic continuum modelling (3D) [Tsang, 1996]
- Discrete fracture network modelling (3D), VAPFRAC [Nordqvist et al, 1995]

In the SITE-94 assessment it was acknowledged that the transport parameters need to be evaluated in an integrated fashion considering the physical characteristics of the fissured rock. If the parameters are treated independently, it may be possible to arrive at unreasonable combinations of parameters, e.g. flow wetted surface and flow rates not possible to obtain in a fissured rock.

For the 3D models the transport parameters were evaluated performing the following steps: solution of steady-state flow, sampling of near-field parameters on canister scale, particle tracking from the individual canisters and interpretation of the canister release curves in terms of effective far-field parameters.

Because the radionuclide transport in the geosphere was calculated with the coupled but simple 1D transport model (CRYSTAL) the results of the 3D hydrogeological site models had to be interpreted in terms of a few effective transport parameters. This was done by dividing the 3D flow field into a set of equivalent stream tubes, each representing flow and transport from a single canister source. For each realization of the flow field and for each canister source the discrete-particle random-walk method of particle tracking provides a distribution of residence times at the surface (interface to the biosphere). An estimate of the effective far-field fluid velocity and the dispersion coefficient was obtained by fitting the 1D advection-dispersion solution to the residence time distribution recorded at the discharge point. In the discrete fracture network models particle tracking results were also used to estimate flow porosity, specific surface area and transport path length.

Two parameters are defined for evaluation and comparison of model results:

$$F = a_r L_{path} / q$$

$$Pe = U L_{path} / D_L$$

where a_r is the flow wetted surface per volume of rock, L_{path} is the transport distance, q is the Darcy velocity, U is the water velocity, and D_L is the longitudinal pore water dispersion.

The F-ratio (F) is a measure of the retardation efficiency in the rock and the Peclet number (Pe) is a measure of the relation between advective and dispersive transport. These two parameter groups describe the main hydrological

influence on radionuclide transport and varying the individual parameters within the groups does not have any effect on the radionuclide release predictions as long as the parameter groups are kept constant. This was also verified by sensitivity analyses using the CRYSTAL radionuclide transport code.

The geosphere transport properties associated with each canister location can thus be characterized in terms of the two parameter groups, (F, Pe) . The spatial variability of the geosphere transport properties was obtained by estimating (F, Pe) for many canister positions in each flow field realization.

Scoping assessment of reactive transport parameters

As complement to the detailed hydrogeological site models a simple scoping evaluation was performed in order to determine uncertainty ranges for water flux (Darcy velocity) and F-ratio [Dverstorp et al., 1996]. Based on simple assumptions of flow field structure and hydraulic driving forces a wide range of plausible water fluxes was determined. Because there was a lack of data for determining the parameters used to give the F-ratio, a set of six different physical models of the pore space geometry in fractures were analyzed to scope the plausible ranges of transport behaviour.

The transport models applied include: a single parallel fracture, a cylindrical tube, multiple parallel fractures, a stepped fracture with aperture varying perpendicular to the direction of the flow, a stepped fracture with aperture varying along the direction of the flow, a parallel fracture filled with uniform spherical particles (representing e.g. a fracture zone with crushed rock). The parameters of all models were chosen such that all models gave the same water flux for a given head gradient, hence the same transmissivity. The transport models were then combined with the water fluxes determined from the simple evaluation of groundwater flux in order to provide a bounding analysis of the uncertainties in the F-ratio.

The predicted F-ratios for Äspö span an extremely wide range, from about 10^8 to 10^{18} s/m. For the Reference Case/Zero Variant source term and geochemistry in SITE-94, F-ratios below 10^{11} s/m corresponds to negligible far-field retardation. Thus, it was not possible to verify the geosphere performance based on the results from the simple evaluation.

Detailed site scale modelling of hydrogeology

The bulk of the hydrogeological predictions was made with the Discrete Feature (DF) site model [Geier, 1996]. This model consists of a 3D, deterministic representation of the SITE-94 geological structure model of Äspö, combined with a stochastic discrete-fracture-network representation of fractures within the repository rock block. The DF model included a large number of variants to evaluate various conceptual and parametric uncertainties in the basic model.

An effective water flux and flow wetted surface area were determined together in conjunction with particle tracking, to ensure that the estimated flow wetted

surface is consistent with the flow field analyzed. The explicit representation of the fractures in the Discrete Feature model, including two simple models of parallel plate fractures, makes estimation of the flow wetted surface straight forward. By means of a simple weighting scheme, fracture surfaces encountered by many particles were given a larger weight when calculating the effective flow wetted surface.

When all model variants were lumped together as an expression of the total spatial variability and (evaluated) uncertainty, the resulting, predicted range of F-ratios was $2 \cdot 10^{10}$ to $5 \cdot 10^{14}$ s/m. The spatial variability of the F-ratios for any particular variant was about 1 to 2 orders of magnitude. Although this represents a reduction of several orders of magnitude, relative to the range predicted by the simple scoping calculations, the predicted F-ratios still span a very wide range, ranging from marginally poor to very good far-field performance.

Independent flow wetted surface estimates

In general the flow wetted surface was not determined independently of the Darcy velocity, instead the F-ratio was evaluated. However, independent estimates of the flow wetted area per volume of rock, a_v , were made for two purposes: evaluation of far-field radionuclide transport based on the Stochastic Continuum site model (that does not provide data on this parameter), and secondly, for the near-field release and transport model. As there are limited data from the Äspö site for estimating the flow wetted surface, results from theoretical modelling with discrete fracture network models were primarily used. In addition, estimates from the scoping assessment, the SITE-94 geological structure model, and from geochemical data were considered.

Although prediction of flow wetted surface was not a specific objective of the simple scoping calculations, values of a_v are easily calculated for the idealized pore geometry models that were analyzed. The range of values of a_v thus calculated extends from 0.0014 to $140 \text{ m}^2/\text{m}^3$. This range is very wide in comparison with ranges estimated with other techniques, which is to be expected due to the broad ranges of uncertainty analyzed. Even lower values were obtained for the cylindrical tube model, but this model was found to be incompatible with reasonable ranges of porosity for a rock mass or fracture zone consisting entirely of such channels.

The Discrete Feature model gave estimates of median values for the flow wetted surface between 0.01 and $0.1 \text{ m}^2/\text{m}^2$ from the site scale particle tracking calculations. The variability between the flow paths from different canisters is 1-2 orders of magnitude. Due to difficulties in determining the bulk or averaging volume of the flow paths, these results cannot be generally used. Thus the flow wetted surface calculated by the Discrete Feature model were only used to calculate F-ratios in that model as described above.

The discrete fracture network model (VAPFRAC) was used to perform synthetic tracer experiments in 3D fracture networks with varying aperture field in the fracture planes using the method of [Dverstorp et al, 1992]. A number of cases

were set up (each with 12 realizations) varying, the location process for fractures, the fracture aperture variance, the aperture correlation length and the fracture discretization. Estimates of a_r ranged from 0.1 to 10 m²/m³, with a median of around 2-3 m²/m³, for all input parameter combinations. The flow wetted surface was most sensitive to changes in aperture variance within the fracture plane.

A simple geometrical estimate of the flow wetted surface was obtained directly from SITE-94 structural model [Voss et al, 1996]. Total area of water conducting structures was found to have a constant value of 0.06 m²/m³ for a large range of averaging volumes. With the assumption that the entire structure is accessible to flow and considering the two sides of the fracture this yields a flow wetted surface of 0.12 m²/m³. The considerably lower value than that predicted by VAPFRAC was said to be likely due to that only site scale structures were included in the geological model.

The flow wetted surface has also been estimated from geochemical data [Glynn and Voss, 1996]. The estimate is based on the assumption that the Rn-222 content in groundwater is related to uranium content in the rock and the flow wetted surface. From Äspö data on uranium content in the rock and radon content in the water a flow wetted surface, a_w , of 3100 m²/m³ water was derived. Using the low end flow porosities from the LPT2 test (10^{-4} - 10^{-3}) a range for the flow wetted surface per volume of rock, a_r , between 0.31 - 3.1 m²/m³ was obtained.

For the far-field radionuclide transport calculations performed with the Stochastic Continuum model and for the near-field radionuclide release and transport calculations, the three values 0.01, 0.1 and 1 m²/m³, were chosen to represent the uncertainty in the flow wetted surface, a_r . However, in the discussion it was questioned whether a single effective value of the flow wetted surface could be used to represent the spatially varying flow wetted area.

Implications for radionuclide transport

In the discussion of conceptual uncertainty it was concluded that the F-ratio had a dominating influence on the peak release rates predicted from the repository. Thus, conceptual uncertainty affecting the parameters making up the F-ratio were of fundamental importance, primarily the water flow rate and the flow wetted surface. These were for the Discrete Feature model the conceptual assumptions regarding pore geometry, and the transmissivity within the features. For the Stochastic Continuum site model, besides the need for independent estimates of flow wetted surface, critical uncertainties were related to the distribution and spatial correlation of the hydraulic conductivity.

4.7 Summary

Parameter values used for the flow wetted surface in performance assessment studies have been based on estimates made using a variety of methods. In

Table 4.2 below a summary of the chosen parameters is made. Over the 13 years which have elapsed since the first study there is no trend of an increased degree of certainty in the values. In most studies ranges of values have been used, spanning 1-2 orders of magnitude. The selected values are usually in the range between 0.01 and 1 m²/m³ of rock. The lowest value, 0.0024 m²/m³ of rock, is used for the crystalline basement of Northern Switzerland and the highest value, 2 m²/m³ rock, is used for a fracture zone in the TVO-92 study.

In two recent performance assessment (TVO-92 and SITE-94) focus has been put on the ratio between the flow wetted surface and the water flux (*F-ratio* = $a_r L_{path}/q$). In Table 4.3 a summary of F-ratios from different assessments is given. For the other safety assessments the F-ratios have been calculated from the far-field parameters. The difference is rather small (a factor of 20) between the highest and lowest value used for the F-ratio in the central or reference case of the different safety assessments. In three assessments (Project 90, TVO-92 and Kristallin-I) almost identical values have been used for the central case. The variation in F-ratio is less than for the assigned value of a_r , where it is a factor of 170 between the highest and lowest value. Also, the difference in the low end value of the F-ratio is relatively small, a factor of 50 between Project 90 and SKB 91. However, the comparison is only approximate since in SKB 91 a probabilistic analysis was made looking at flow paths from 88 positions in the repository in 500 realizations. From some of the starting positions travel times were less than 10 years in some of the realizations.

Table 4.2 Summary of values for the flow wetted surface used in performance assessment studies.

Study Year	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]
KBS-3 1983	bore hole measurements of hydraulic fracture frequency	0.4	4000
SKB-91 1992	Tracer experiments [Abelin et al., 1987]	0.2 - 2 (possibly up to 20)	
	Observations of channel widths [Moreno and Neretnieks, 1991]	0.006 - 0.4	
	Chosen for safety assessment	0.1 (0.01 - 0.5)	1000
Project-90 1991	DFN-model calibrated to field experiment [Dverstorp, 1991]	0.001 - 5	
	Chosen for safety assessment	0.01	
TVO-92 1992	Estimates for intact rock	0.04- 0.08	
	Estimates for disturbed rock	0.5 - 2	
	Estimates for fracture zones	1.2 - 2	
Kristallin-I 1994	Assessment of water bearing features	0.0024-0.17	1000
SITE-94 1996	Simple scoping calculations [Dverstorp et al, 1996]	0.0014-140	
	Discrete feature model [Geier, 1996]	0.01 - 0.1	
	DFN-model [Nordqvist et al, 1995]	0.1 - 10	
	Observed area of site-scale structures [Voss et al, 1996]	0.12	
	Uranium content and radon concentration [Glynn and Voss, 1995]	0.31 - 3.1	3100
	Chosen for safety assessment*	0.01, 0.1, 1	

* Only used for the Stochastic continuum modelling (Section 3.6)

Table 4.3 Summary of F-ratio ($F=aL/q$) used in various safety assessments.

Study	a_r	L_{path} [m]	q [$\text{m}^3/(\text{m}^2, \text{a})$]	F-ratio[a/m]		
				Low	Reference	high
KBS-3	0.4	100	10^{-4}		$4 \cdot 10^5$	
SKB 91	0.1	^{a)}	10^{-3} ^{b)}	10^4 ^{c)}	10^5 ^{d)}	10^7 ^{e)}
Project 90	0.01, 1	200	$10^{-4}, 10^{-2}$	$2 \cdot 10^2$	$2 \cdot 10^4$	$2 \cdot 10^6$
TVO-92	$0.04 \cdot 2$ ^{f)}	400 ^{f)}	$10^{-4} - 10^{-2}$ ^{f)}	$4 \cdot 10^3$	$2 \cdot 10^4$	$1 \cdot 10^5$
Kristallin-I	0.0024-0.066	200	$2.5 \cdot 10^{-5}$		$2 \cdot 10^4$	$5 \cdot 10^5$
SITE-94	0.01, 0.1, 1 ^{g)}	500	$10^{-5} - 2 \cdot 10^{-2}$	$7 \cdot 10^2$ ^{h)}	$7 \cdot 10^4$ ^{h)}	$6 \cdot 10^6$ ^{h)}

Notes

a_r flow wetted surface per volume of rock [m^2/m^3]

L_{path} migration path length [m]

q water flux [$\text{m}^3/(\text{m}^2, \text{a})$]

- a) not evaluated, most frequent groundwater travel time ≈ 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-ratios chosen from an analysis of different flow paths from the repository to the biosphere
- g) only used for the Stochastic continuum modelling (Section 3.6)
- h) F-ratio evaluated from site-scale flow and transport calculations in discrete fracture modelling

5 Discussion and recommendations

In a number of safety analyses the effective area available for contact between the flowing water and the rock has been found to be crucial for the retardation of sorbing radionuclides. This has generally been described by the parameter flow wetted surface, which gives the specific contact area between the flowing water and the rock per volume of rock, or alternatively, per volume of flowing water. Unfortunately, this parameter is not readily measured, instead it must be assessed through indirect methods. In recent studies (eg TVO-92 and SITE-94) focus has been put on the ratio between the total surface of a flow path and the water flow rate in the path. This integrated parameter has been shown to have a dominating influence on the peak release predicted from a spent fuel repository.

In the ongoing discussion on the most suitable model for incorporate the flow wetted surface in safety assessment models, there is a trend towards considering the ratio between the flow wetted surface and the water flow rate to be the more appropriate parameter for describing the efficiency of retardation in the rock than the flow wetted surface. However, there is still some controversy about the best methods to estimate this ratio and to what extent the flow wetted surface/water flux ratio can be treated as an intrinsic material property and to what extent it will depend on the flow situation and the boundary conditions.

Various methods have been used to make estimates of the flow wetted surface, tracer tests, tunnel and borehole investigations, geochemical studies, as well as theoretical modelling. The variability between the estimates is usually very large, often 2 to 3 orders of magnitude. The differences in the results are partly due to the method used and partly to different properties of the rock. However, the values used in safety assessments usually fall within the range 0.01-1 m²/m³ rock. It is not likely that any single method will give sufficient confidence in the estimates of the flow wetted surface. Instead, estimates using several methods need to be intercompared.

The long-term research needs to address the uncertainty concerning the flow wetted surface both on a detailed scale as well as on a larger scale. On the detailed scale questions concerning the actual flow path geometries, the importance of stagnant zones of water and how these affect the actual estimates of the flow wetted surface within a fracture, needs to be addressed. On the larger scale, the methods to assess the effective flow wetted surface along flow paths needs to be developed. Furthermore, the variability of the effective flow wetted surface for large scale flow paths in relation to the water flow rate needs to be further studied. Of special interest is the possibility of having flow paths with considerably smaller ratio flow wetted surface to water flux, as such flow paths can lead to considerably faster transport through the geosphere. A lot of effort is

presently put on these issues both in the form of experiments to better characterize the rock and understand the details of the flow as well as theoretical modelling to understand the implications on radionuclide transport.

Another issue which has presently not been much investigated is the persistence of flow paths, considering the long perspective that needs to be considered for radionuclide transport in the geosphere. Rock stresses and thereby fracture apertures will be affected by glaciations, geochemical processes can lead to the filling of fractures, etc. Studies of geological evidence of surface interactions may prove valuable in the study of long-term changes.

A combination method that seems worthwhile to investigate further is the combination of tracer tests and heat transfer tests. The transport of heat would in this case simulate the transport of a reactive tracer. The conditions for such tests must be further studied, eg the temperature differences should not be so large that they significantly change the flow, but still large enough to be detected.

Of special interest are methods that can be used to estimate the ratio between the total surface of a flow path and the water flow rate in the path. This integrated parameter has been shown to have a dominating influence on the peak release predicted from a spent fuel repository. This requires a detailed understanding of the flow situation within the fissured rock. The question of how the ratio between flow wetted surface and water flux varies along the different flow paths from the repository should be addressed in future safety assessments.

In conclusion, the following recommendations can be given:

- At present no individual method can be selected that satisfies all requirements concerning giving relevant values, covering relevant distances and being practical to apply. Instead a combination of methods must be used.
- The long-term research should address both the detailed flow within the fractures and the effective flow wetted surface along the flow paths and its spatial variability. There is still a lack of knowledge on how the flow and transport in fractured rock really take place.
- In the safety assessment modelling focus should be put on the ratio between flow wetted surface 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.
- Further development is needed of methods for assessing the flow wetted surface by evaluating the effect of interactions at the flow wetted surface, eg sorption of tracers, release of radon or the analogues using exchange of heat.

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List of Notations

a_r	flow wetted surface per volume of rock	$[\text{m}^2/\text{m}^3]$
a_w	flow wetted surface per volume of water	$[\text{m}^2/\text{m}^3]$
D_L	longitudinal dispersion	$[\text{m}^2/\text{a}]$
F	Parameter group representing retardation capacity in rock	$[\text{a}/\text{m}]$
L	length of channel	$[\text{m}]$
L_{path}	length of flow path or transport distance	$[\text{m}]$
Q	flow rate in channel	$[\text{m}^3/\text{a}]$
q	water flux (Darcy velocity)	$[\text{m}^3/(\text{m}^2, \text{a})]$
U	water velocity	$[\text{m}/\text{a}]$
W	width of channel	$[\text{m}]$
W'	total channel width per rock cross-section area	$[\text{m}/\text{m}^2]$
x_1	channel width	$[\text{m}]$
x_2	half-distance between channels	$[\text{m}]$
y_1	half-aperture of features	$[\text{m}]$
y_3	half-distance between features	$[\text{m}]$
ϵ_f	flow porosity	$[-]$
γ	total trace length of features intersected by plane	$[\text{m}/\text{m}^2]$

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1977-78

TR 121

KBS Technical Reports 1 – 120

Summaries

Stockholm, May 1979

1979

TR 79-28

The KBS Annual Report 1979

KBS Technical Reports 79-01 – 79-27

Summaries

Stockholm, March 1980

1980

TR 80-26

The KBS Annual Report 1980

KBS Technical Reports 80-01 – 80-25

Summaries

Stockholm, March 1981

1981

TR 81-17

The KBS Annual Report 1981

KBS Technical Reports 81-01 – 81-16

Summaries

Stockholm, April 1982

1982

TR 82-28

The KBS Annual Report 1982

KBS Technical Reports 82-01 – 82-27

Summaries

Stockholm, July 1983

1983

TR 83-77

The KBS Annual Report 1983

KBS Technical Reports 83-01 – 83-76

Summaries

Stockholm, June 1984

1984

TR 85-01

Annual Research and Development Report 1984

Including Summaries of Technical Reports Issued during 1984. (Technical Reports 84-01 – 84-19)

Stockholm, June 1985

1985

TR 85-20

Annual Research and Development Report 1985

Including Summaries of Technical Reports Issued during 1985. (Technical Reports 85-01 – 85-19)

Stockholm, May 1986

1986

TR 86-31

SKB Annual Report 1986

Including Summaries of Technical Reports Issued during 1986

Stockholm, May 1987

1987

TR 87-33

SKB Annual Report 1987

Including Summaries of Technical Reports Issued during 1987

Stockholm, May 1988

1988

TR 88-32

SKB Annual Report 1988

Including Summaries of Technical Reports Issued during 1988

Stockholm, May 1989

1989

TR 89-40

SKB Annual Report 1989

Including Summaries of Technical Reports Issued during 1989

Stockholm, May 1990

1990

TR 90-46

SKB Annual Report 1990

Including Summaries of Technical Reports Issued during 1990

Stockholm, May 1991

1991

TR 91-64

SKB Annual Report 1991

Including Summaries of Technical Reports Issued during 1991

Stockholm, April 1992

1992

TR 92-46

SKB Annual Report 1992

Including Summaries of Technical Reports Issued during 1992

Stockholm, May 1993

1993

TR 93-34

SKB Annual Report 1993

Including Summaries of Technical Reports Issued during 1993

Stockholm, May 1994

1994

TR 94-33

SKB Annual Report 1994

Including Summaries of Technical Reports Issued
during 1994.

Stockholm, May 1995

1995

TR 95-37

SKB Annual Report 1995

Including Summaries of Technical Reports Issued
during 1995.

Stockholm, May 1996