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Description of the transport mechanisms and pathways in the far field of a KBS-3 type repository

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ABSTRACT

The main purpose of this document is to serve as a reference document for the far field radionuclide transport description within SKB 91. A conceptual description of far field transport in crystalline rock is given together with a discussion of the application of the stream tube concept. In this concept the transport in a complex three-dimensional flow field is divided into a number of imaginary tubes which are modelled independently. The stream tube concept is used as the basis for the radionuclide calculations in SKB 91. Different mathematical models for calculating the transport of radionuclides in fractured rock are compared: advection dispersion models, channeling models and network models. In the SKB 91 project a dual-porosity continuum model based on the one dimensional advection-dispersion equation taking into account matrix diffusion, sorption in the rock matrix and radioactive chain decay.

Furthermore, the data needed for the transport models is discussed and recommended ranges and central values are given.

CONTENTS

1 BACKGROUND AND INTRODUCTION

SKB 91 is a site-specific performance assessment study for a repository for spent fuel in crystalline rock. The main goal of the project is to visualize and quantify how different geological parameters affect the long-term safety of the repository.

The site of interest is the Finnsjön area in northern Uppland where extensive field investigations have been carried out since 1977. The two dominating geological structures are the highly conductive, gently low-dipping fracture zone 2 and the nearly vertical zone 1, called the Brändan zone. The latter divides the Finnsjön Rock Block into two parts, the northern and the southern part. The hypothetical repository, which is of a KBS-3 type, will be placed below the almost horizontal zone 2 in the northern part of the area. This is motivated by the general better knowledge of the northern part, as compared to the southern, as well as the relatively stagnant groundwater conditions below zone 2. An overview of the geological and the geohydrological conditions at the Finnsjö site is given in Ahlbom et al. [1991].

The main purpose of this document is to serve as a reference document for the far field radionuclide transport description within SKB 91. A conceptual description of far field transport in crystalline rock will be given as well as a discussion of the different transport parameters. For details about computer codes and the data used in the SKB 91 calculations the reader is referred to other documents.

The stream tube concept for radionuclide transport will be used as the basis for radionuclide transport calculations. The stream tube model is based on particle tracks generated by a groundwater flow model. The starting points of the different stream tubes are positioned at the periphery of the repository, or the near field. The stream tube concept and the division of the repository into stream tubes will be discussed in the report.

Finally, it is assumed that a three-dimensional flow field is given by a hydrology model. A Monte Carlo simulation code, HYDRASTAR [Norman, 1991], will be used for the groundwater flow calculations. The goal is to take account of the spatial variability of the rock properties since these are expected to be of great importance to the groundwater flow situation. The geohydrology model will not be further discussed in this document.

2 FLOW AND TRANSPORT IN FRACTURED ROCK

In the Swedish KBS-3 concept, the repository for spent nuclear fuel is located deep in the crystalline bedrock away from larger fracture zones. In these zones, which may be very long and extend to great depth, the rock is considerably more fissured. The widths of the fracture zones range from a few meters to several hundred meters. However, also the rock between the larger fracture zones contains smaller fractures of which some are water bearing. The tunnels and shafts of the repository will be intersected by a number of such smaller fractures. If the copper canisters containing the spent fuel fail, radionuclides will be released through the surrounding backfill material and may be transported by the groundwater in these smaller fissures to the larger fracture zones. Radionuclides may eventually reach the biosphere, for example if they reach a fracture zone with an upward water movement.

Investigations of water flow in crystalline rock indicate that the flow is very unevenly distributed. Only a part of the visible fractures carry any water and only a few of these are responsible for the largest parts of the observed flow rates. It has also been found that the flow is located to certain pathways within the fractures. This has been noted from inspections of excavated tunnels where it can be seen that water emerges in narrow spots in fractures and fracture intersections [Neretnieks et al., 1987]. These observations together with results from tracer migration tests [Abelin et al., 1987] has lead to the development of the conceptual model of channeling. The idea is that the water flows in quite widely separated channels, which may extend for considerable distance without significantly intersecting other channels.

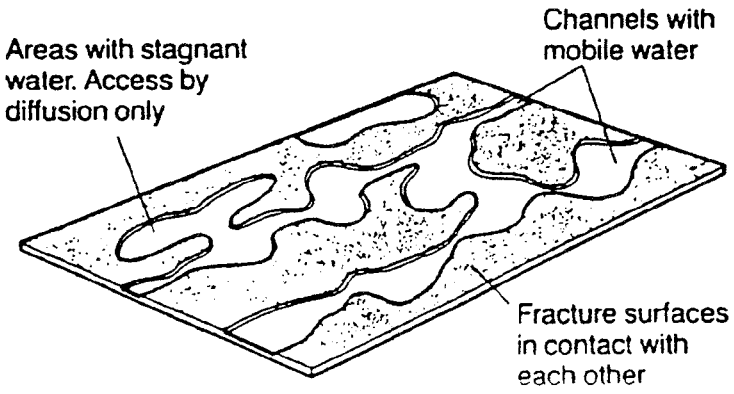

Figure 2-1 Conceptual picture of channels with mobile water within a fracture plane formed between the areas of contact of the surfaces [Rasmuson and Neretnieks, 1986b]

Due to variations in fracture aperture the water is restricted to flow in only a part of the fracture plane, see Figure 2-1. In some locations, the two rock surfaces will be in direct contact or the fracture is closed by fracture filling material, giving no access to the water, and in other locations, areas with stagnant water will form. The actual shape of the channels or flowpaths will vary, at some locations they may be narrow tubes and at other locations they may more resemble planar slits. Due to the limited area of the fracture planes with substantial water flow it is possible that two fractures may intersect without or with incomplete mixing of the water between the channels in the two fracture planes.

The actual nature of the flowpaths within the fractured rock will effect the radionuclide transport for several reasons. Firstly, the size of the contact area between the flowing water and rock surface is crucial for the diffusion into the rock matrix and for the sorption of dissolved species on the rock. Matrix diffusion and subsequent sorption onto inner surfaces is by far the most important retardation mechanism for sorbing nuclides [Neretnieks, 1989]. Secondly, the flow path connectivity is of importance for the residence time distribution and thereby for the dispersion of radionuclides. Additionally, the flow path dimensions will of course be of importance for such entities as migration distance and residence time of water.

Dispersion will give rise to a spreading of the concentration pulse and thereby a lowering of the maximum release rate for narrow peaks. However, the spreading may also lead to an earlier breakthrough, which may lead to an increased release of radionuclides with a radioactive half-life of the same magnitude as the travel time, due to the decreased time for radioactive decay.

3 TRANSPORT MODEL

3.1 Stream tube concept

3.1.1 General

A stream tube is an imaginary tube defined as a volume enclosed by a surface made up by a set of streamlines. No fluid can pass through its walls. This is a very useful concept because by dividing a very complex three-dimensional flow field into a number of stream tubes, the transport of solutes in every stream tube can be described independently of the other stream tubes. The stream tube will contain the fractured rock with its water bearing fractures. In a stream tube which has a large cross-section compared to pores or channels of a porous or fractured rock, there will be little fluid passing over the boundaries of the stream tube and the error introduced by neglecting this small flow through the walls, is deemed to be permissible.

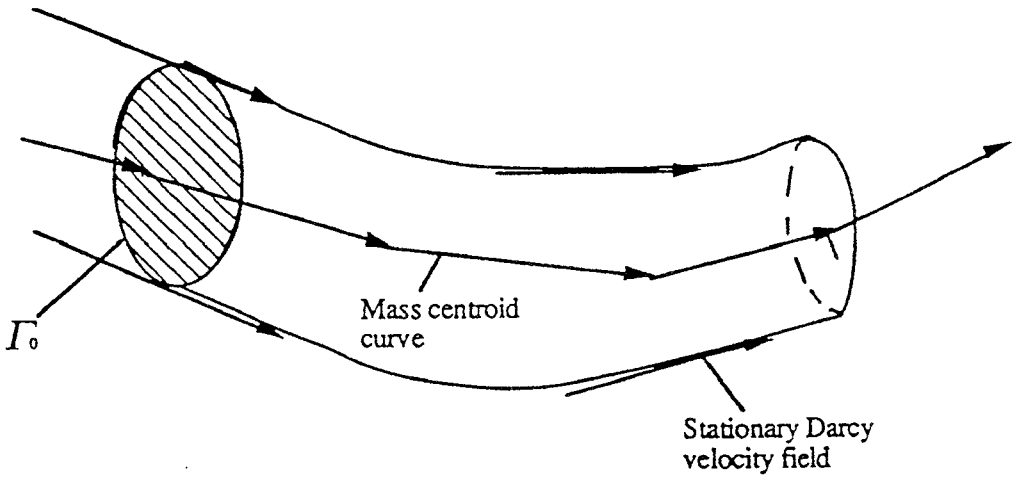

Figure 3-1 Conceptual picture of stream tube [Norman and Kjellbert, 1990]

As no water will pass over the stream tube boundaries, the water flow rate through a cross-section of the stream tube (m^3/s) will be the same everywhere along the tube. However, the water flux ($m^3/m^2,s$), often called the Darcy velocity, may vary along the tube. Due to the conservation of mass a variation in flux will lead to a variation in the cross-sectional area of the stream tube. A high flux will correspond to a small cross-sectional area and a low flux to a large cross-sectional area. In order to determine the cross-section area of the stream tube, the water fluxes along the tube and the water flow rate in it must be known.

Much of the subsequent discussion is associated with the averaging of hydraulic properties in stream tubes. A basic assumption used is that no net transversal mass transport takes

place in the stream tube (i. e. no diffusive or dispersive exchange between stream lines), which allows for transversal mass flow averaging to be used. Water parcels moving inside the tube will be represented by their collective center of gravity.

3.1.2 Division of flow from repository into stream tubes

One of the purposes of the discretization technique using stream tubes is to make it possible to take into account the release of radionuclides from the near field of the entire repository. To that end, the repository is divided into a number of parts each encompassed by a stream tube. Figure 3-2 gives a schematic picture of stream tubes going from the repository to the ground surface. A typical number of stream tubes would be 100, each thus covering a cross-sectional area of 10 000 m^2 at the repository level. This is deemed to be a reasonable size to ensure that the transport over the stream tube boundaries is small compared to the flow in the stream tube. Each stream tube will then contain 50-60 waste canisters, which is considered to be sufficient for obtaining an average of the release of nuclides into the stream tube.

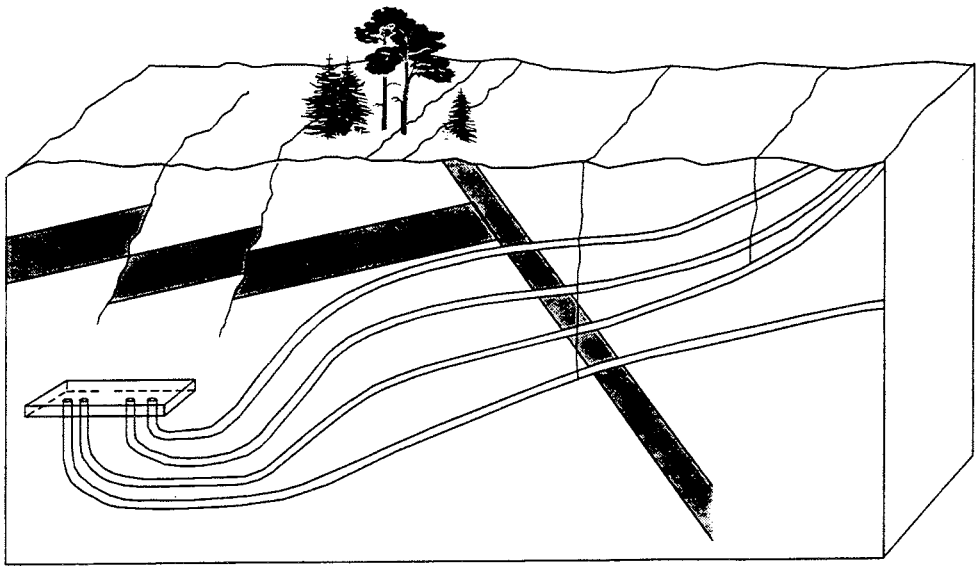

Figure 3-2 Schematic picture of stream tubes going from the repository to the ground surface.

In the application of the stream tube concept for the SKB 91 project the stream tubes are generated by a particle tracking technique. The starting positions of the particles are distributed over the repository, two for every second deposition drift, see Figure 3-3. The travel time to the ground surface for a released particle is assumed to be representative for a segment containing the neighboring canisters. This segment will constitute the initial cross-section of the stream tube. In this way all canisters in the repository will be

distributed between roughly 88 stream tubes. However, the initial cross-sectional area of these stream tubes or the number of canisters included may not necessarily be the same for all stream tubes.

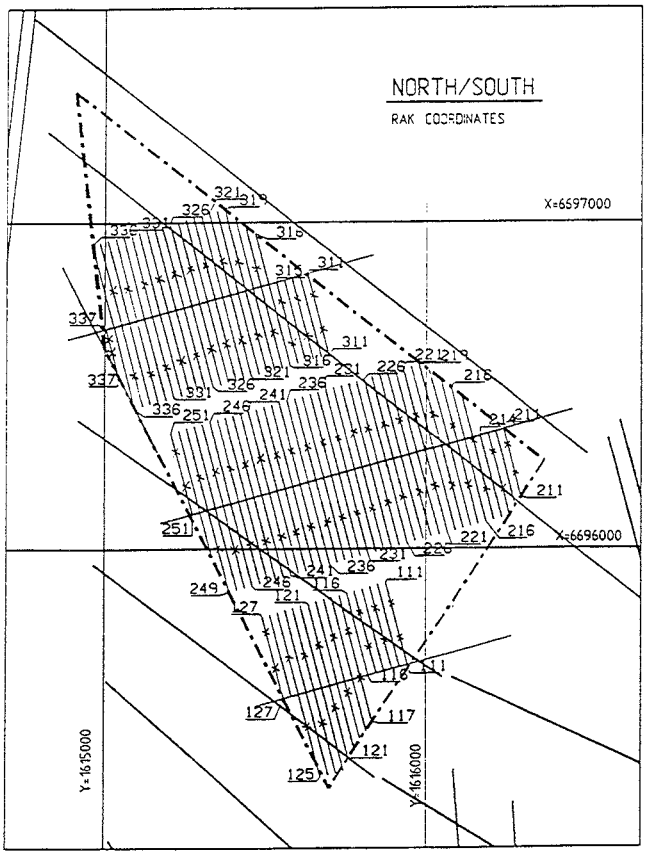

Figure 3-3 Deposition drifts with starting positions of the particles [Ageskog and Sjödin, 1991]

The near field transport model used in SKB 91 uses the water flux in each segment as input for the computation of the radionuclide release rate. In the case of late canister failure is it assumed that the radionuclide release is identical for each canister within a segment. However, if a segment contains a canister with an assumed initial failure, only the radionuclide release from that canister will be considered.

The advantage with this application of the stream tube concept is that the entire repository is covered. The drawback is the averaging out of the differences between the individual canisters in each stream tube. It may be noted that within the stream tube, the flow and transport modelling at the local scale can be done by porous media models but also with fracture network or channel network models. The latter models makes it possible to treat the flow past every canister individually. Some of the canisters may not be intersected by any flowing channels and others may be hit by "high" flow channels. However, this local scale transport modelling has not been performed within the SKB 91 project.

3.2 Concepts of transport in stream tubes

The use of the stream tube concept is based on the assumption that the main mechanism for transport of dissolved radionuclides is by the flowing groundwater. The stream tube will encompass a flow domain consisting of both rock and flowing water. No presumptions are made of the detailed characteristics of rock or of the types of flow paths within this flow domain. It could be porous rock, fissured rock, or rock with extreme channeling. Assumptions of the type of flow paths will instead be used when determining the input parameters for the radionuclide transport model.

The stream tube concept greatly facilitates the modelling of the radionuclide transport. Instead of having to describe the radionuclide transport in three dimensions using three-dimensional flow fields obtained in hydrology calculations, a number of one-dimensional calculations is performed. Naturally, such a procedure implies a number of simplifying assumptions. By definition there is no flow and advective transport over the boundaries of a streamtube. Since each stream tube is modelled independently, no consideration can be taken to any interaction between stream tubes. Thus, it is assumed that there will be no mixing of water and thus no dispersive mixing of the transported radionuclides between stream tubes. However, dispersive mixing along the stream tube can be described. Furthermore, it is assumed that there is no diffusive transport of radionuclides between stream tubes.

3.2.1 Advection-dispersion model

The application of the advection-dispersion model to the transport in stream tubes is based on the continuum approach, i.e. an averaging of the transport properties over a larger volume is made. The rock in this volume is assumed to have the properties of a continuous medium. In many applications different parts of the rock are modelled as two separate continua, e.g. the fissures with flowing water and the microfissures of the matrix with stagnant water. This is sometimes referred to as the dual porosity approach.

The classical advection-dispersion equation has been extensively used for porous media where it can be assumed that the dissolved radionuclides move with the average velocity of the water and that the variation of the radionuclide transport rate around the average velocity is a random process similar to molecular diffusion. This process is often referred to as Fickian dispersion. The advection-dispersion model may also be applied to fissured media using the flux (Darcy velocity) or a water velocity derived from the flux and the flow porosity.

The advection-dispersion equation may then be written as:

$$\varepsilon_f R \frac{\partial c}{\partial t} = \varepsilon_f D_L \frac{\partial^2 c}{\partial z^2} - u_0 \frac{\partial c}{\partial z} \qquad \textbf{(3-1)}$$

where:

c is the radionuclide concentration in the pore water
t is time

z	is distance in the flow direction
R	is the retardation factor
ε_f	is the flow porosity
D_L	is the dispersion coefficient
u_0	is the water flux (Darcy velocity = water flow rate per unit area)

In the case of transport in fissured rock, the dispersion is largely due to velocity variations between the flow in different water flow paths. This will greatly exceed the hydrodynamic dispersion due to velocity differences within a single flow path. Molecular diffusion within the flowing water will have a very small effect on the spreading of the radionuclides. On the contrary, molecular diffusion will reduce dispersion arising from velocity variations within a flow path since it will tend to even out the lateral (transversal) concentration differences [Neretnieks, 1983].

In the advection-dispersion model, the dispersion coefficient is implicitly assumed to be independent of the accumulated distance in the flow direction. This would be the case if there was a frequent mixing of water from different flow paths. However, in crystalline rock at large depths the fractures are usually far apart and long distances are needed in order to have a sufficient mixing. The degree of mixing needed will also depend on the variability of the flow rates in the different flow paths. If the spread in water flow rate between different flow paths is large the advection-dispersion model will not very well describe the dispersion in fractured rock even at considerable transport distances [Rasmuson, 1985].

In Equation 3-1 it is implicitly assumed that D_L does not depend on location, meaning that it is independent of z. This is a common assumption and there is no data to support that this should not be the case in a medium with constant properties. However, the dispersion coefficient D_L has been found to depend on the water velocity, and can be written $D_L = \alpha \cdot u$. Here α is the dispersion length.

Field and laboratory experiments in fractures and in fractured rocks indicate that the longer the flow path is, the larger is the dispersion coefficient and the dispersion length. Seemingly the dispersion length is proportional to the length of the flow path. This violates one of the basic assumptions in the advection- dispersion model. The experimental breakthrough curves can be fitted very well with models and can thus also be used for predictions if only the dispersion length is chosen such that the distance effect is accounted for.

When the dispersion length is proportional to the length of the flow path this also means that α is a multiple of the path length Z. The commonly used dimensionless entity, the Peclet number, Pe relates these entities by:

$$Pe = Z/\alpha = Z \cdot u/D_L$$

where:

Z is the migration distance
u is the water velocity

In the present application it is thus practical to describe the dispersion by choosing a constant value of Pe which then would not depend on the path length.

Retardation mechanisms

The transport of dissolved radionuclides in the flowing water may be retarded in relation to the water velocity. This may be due to sorption onto the solid surfaces - *surface sorption* - or due to diffusion of the radionuclides into the porous rock matrix - *matrix diffusion*. The diffusion into the matrix also gives access to the large inner surfaces of the rock matrix where the radionuclides may sorb.

Surface sorption

The surface sorption is commonly modeled as an instantaneous reversible equilibrium process described by a surface sorption coefficient, K_a. The retardation factor due to surface sorption can then be described by:

$$R = 1 + K_a \cdot a_W \qquad \textbf{(3-3)}$$

where a_W is the contact area between the flowing water and the solid in m^2/m^3 of flowing water, hereafter referred to as *the flow-wetted surface*.

It can be shown that for radionuclides with non-negligible surface sorption, the nuclide velocity in the rock will in practice be independent of the linear velocity of the water in the fractures [Neretnieks et al., 1987]. The nuclide velocity is then determined primarily by the water flux (Darcy velocity), the surface sorption coefficient and the contact area between the flowing water and the fracture surfaces. It may in this case be more convenient to use the flow-wetted surface per unit volume of rock, a_R. This is related to a_W by:

$$a_R = a_W \cdot \varepsilon_f \qquad \textbf{(3-4)}$$

The entity a_R can be estimated from observations of the number of fractures in the rock and from the fraction of the fractures which conduct water.

Matrix diffusion

The Swedish bedrock has been found to have a continuous system of microfissures between the crystals in the rock matrix. These micropores are filled with practically stagnant groundwater. Radionuclides present in the flowing water in the fractures can diffuse by molecular diffusion into the pore water of the rock matrix. At a later stage the radionuclides may diffuse out of the matrix back to the flowing water of the fracture. This effect may give an important retardation of sorbing as well as for non-sorbing radionuclides. For the sorbing radionuclides the large inner surfaces available of sorption inside the rock matrix will be important.

The retardation due to matrix diffusion will in this case not be constant in space or time, but will seem to increase with time, since the penetration depth will change with contact time. It has been shown that the rock volume that can be accessed by diffusion during contact times of hundreds of years may have a considerably larger retardation effect than the surface sorption [Neretnieks, 1980]. The penetration depth will be very small for strongly sorbing nuclides, but in this region the concentration of sorbed radionuclides will be very high and the total amount of radionuclides residing in this region will be large. Thus, the major part of the sorption capacity of the rock matrix will not be available. In the case of matrix diffusion, as for surface sorption, the contact area between the flowing water and the fracture walls will be one of the most important parameters, whereas the flow porosity will have negligible influence for most of the sorbing radionuclides. For non-sorbing nuclides or when the fractures are very close to each other all the rock volume may be equilibrated.

Applications to stream tubes.

With the stream tube concept account can be taken to the multidimensional nature of the radionuclide transport. The important parameters for the radionuclide transport is the water flux, the flow-wetted surface per unit volume of rock and the volume of rock matrix available for sorption as a function of penetration depth into the matrix.

The stream tubes determined by the hydrological model have been calculated with a particle tracking technique and gives the accumulated distance of a particle as a function of time or, alternatively, the water flux as a function of distance along the stream tube. The water flux can be converted into a velocity of the water in the fractures using the flow porosity of the rock. This conversion can either be made in the hydrological model or separately afterwards. By integrating the inverse of the water velocity over the stream tube length the groundwater travel time is obtained. However, for later use of this information in the transport models also the flow-wetted surface influences the transport and the flow porosity influences both water velocity, u, and flow-wetted surface, a_W. Thus, the information on flow porosity variation along the streamtube must also be transferred to the transport model. As noted earlier the sorbing nuclide residence time is in practice independent of variations in water velocity caused by variations in porosity. It is determined by the flow-wetted surface and the water flux. It would thus be much simpler to use the water flux directly in the transport models, not having to keep track of flow porosity variations. The latter is a poorly known entity anyway.

In the modelling of the surface sorption and the matrix diffusion it is necessary to know the available fracture surface area as a function of volume of the rock, a_R or as a function of volume of flowing water, a_W if the flow porosity is known.

Model used in the KBS-3 study

In the KBS-3 study [KBS, 1983] the specific surface was determined from observations in nature of spacing between water bearing fractures. In this study the description of the actual flow paths was treated in a simplified fashion. A constant average water flow rate and an average or shortest length of the migration path was used. In essence the whole repository was encompassed in one stream tube. Retardation of the radionuclides by

matrix diffusion and sorption on inner surfaces was accounted for. Dispersion was modeled as a Fickian process.

The modeled domain consisted of a straight tube containing both the water bearing fractures and the blocks of rock. The tube had a constant cross-sectional area and the water velocity in the tube was constant. The cross-sectional area of the tube was determined by the Darcy velocity and the water flow rate. The one-dimensional advection-dispersion model including the effects of matrix diffusion was used. Thus, the concentration in the water bearing fractures and in the pores of the matrix was calculated explicitly.

Neglecting retardation due to surface sorption, a radionuclide in a radioactive decay chain, the concentration in the flowing water of the fractures c_i, can be described by [Neretnieks and Rasmuson, 1984]:

$$\frac{\partial c_i}{\partial t} = -u \frac{\partial c_i}{\partial z} + D_L \frac{\partial^2 c_i}{\partial z^2} + a_W D_e \left.\frac{\partial c_{p,i}}{\partial x}\right|_{x=0} - \lambda_i c_i + \lambda_{i-1} c_{i-1} \qquad \textbf{(3-5)}$$

where:

c_i is the concentration of nuclide i in the flowing water
$c_{p,i}$ is concentration nuclide i in the pores of the rock matrix
u is the water velocity
z is the distance along the migration path
D_e is the effective diffusivity in the rock matrix
λ_i is the radioactive decay constant for nuclide i
x is the distance into the rock from the flow-wetted surface

For the concentration in the pores of the rock matrix, c_p, the following is obtained:

$$\varepsilon_p R_i \frac{\partial c_{p,i}}{\partial t} = D_e \frac{\partial^2}{\partial x^2} c_{p,i} - \lambda_i \varepsilon_p R_i c_{p,i} + \lambda_{i-1} \varepsilon_p R_{i-1} c_{p,i-1} \qquad \textbf{(3-6)}$$

where:

R_i is the matrix retardation factor ($R_i = 1 + K_d \rho (1 - \varepsilon_p)/\varepsilon_p$)
ε_p is the diffusion porosity of the matrix
K_d is the sorption coefficient
ρ is the solid density of the rock

These equations are connected through the fourth term in Equation 3-5.

Surface sorption on the fracture surfaces was not included in the KBS-3 calculations because the effects were considered negligible compared to the uptake in the matrix.

Model used in the SKB 91 study

In the SKB 91 project, the FARF31 model [Norman and Kjellbert, 1990] is used to calculate the transport along each stream tube. This dual porosity continuum model is based on the one dimensional advection-dispersion equation taking into account matrix diffusion, sorption in the rock matrix and radioactive chain decay. The matrix diffusion is assumed to take place in one dimension. The model is based on flux-averaged quantities of concentration, water velocity, dispersivity and the exchange rate between the flowing water and the pores of the rock matrix. The distance in the flow direction, z, is transformed into accumulated groundwater travel time, ζ. In the present applications a constant flow porosity has been used.

The implementation used in FARF31 requires that the coefficients are constant along the stream tube. Thus, when applying FARF31 to a stream tube with a varying water flux, constant effective parameters must be derived by suitable averaging techniques. The coefficient of the dispersive term (the second term on the right hand side of Equation 3.5) is formulated in terms of groundwater travel time and Peclet number instead of using the dispersion coefficient. FARF31 can thus use groundwater travel times computed by the HYDRASTAR model. This is based on the approximation that the coefficient of the dispersive term can be averaged along the stream tube, yielding the ratio of the residence time and an effective Peclet number.

The averaging of the parameters associated with the matrix diffusion is more complicated. It is assumed that at each point of the interface between the flowing water and the rock matrix there is a one dimensional tube of finite length perpendicular to the rock surface where diffusion takes place. Diffusion tubes at different points can have different lengths, but are not allowed to intersect. The averaging involves weighting on both the surface area between the flowing water and the rock, the length of the one dimensional diffusion tubes, as well as the water flux [cf. Norman and Kjellbert, 1990]. The procedures to determine an average effective flow-wetted surface is not yet developed, see Section 3.3.4. However, as noted above, this difficulty does not arrive if the problem is formulated in terms of flux instead of velocity for sorbing nuclides.

The equations on which FARF31 are based, and which can be shown to be valid also for non-straight stream tubes with varying cross-section [Norman and Kjellbert, 1990], are in summary:

$$\frac{\partial c_i}{\partial t} = -\frac{\partial c_i}{\partial \zeta} + \frac{t_w}{Pe}\frac{\partial^2 c_i}{\partial \zeta^2} + a_W D_e \left.\frac{\partial c_i}{\partial x}\right|_{x=0} - \lambda_i c_i + \lambda_{i-1} c_{i-1} \qquad \textbf{(3-7)}$$

$$R_i \frac{\partial c_{p,i}}{\partial t} = D_e \frac{\partial^2 c_{p,i}}{\partial x^2} - R_i \lambda_i c_{p,i} + R_{i-1} \lambda_{i-1} c_{p,i-1} \qquad \textbf{(3-8)}$$

under the following initial and boundary conditions:

at $t = 0$ $\qquad c_{p,i} = 0$ and $c_i = 0$

when $\zeta \rightarrow \infty$ $\qquad c_i = 0$

the inlet flow is given by:

$$F_{in}^{i}(t) = Q_{tube}\left(c_i(\zeta,t) - \frac{t_w}{Pe}\frac{\partial c_i(\zeta,t)}{\partial \zeta} \right)\Bigg|_{\zeta=0} \quad \textbf{(3-9)}$$

The boundary conditions for the diffusional tubes are:

$$\left.\frac{\partial c_{p,i}}{\partial x}\right|_{x = x_0} = 0 \quad \textbf{(3-10)}$$

$$c_{p,i}(x,\zeta,t)\big|_{x=0} = c_i(\zeta,t) \quad \textbf{(3-11)}$$

The output flux of radionuclide i from the stream tube is given by:

$$F_{out}^{i}(t) = Q_{tube}\left(c_i(\zeta,t) - \frac{t_w}{Pe}\frac{\partial c_i(\zeta,t)}{\partial \zeta} \right)\Bigg|_{\zeta=t_w} \quad \textbf{(3-12)}$$

where:

ζ	is the distance in the flow direction expressed in terms of ground water travel time
$c_{p,i}$	is the surface and flux-averaged concentration of radionuclide i in the pore water
c_i	is the flux-averaged concentration in the flowing water
t_w	is the groundwater travel time over the entire flow path
a_W	is the surface area between the flowing water and the rock per unit volume of flowing water
x	is the penetration depth in the matrix
x_0	is the maximum penetration depth in the matrix
Q_{tube}	is the flow rate in the stream tube

The transport equations are solved analytically in the Laplace plane. These solutions are then numerically inverted to the time domain.

3.2.2 Channeling model

The effect of extreme channeling has been evaluated by discrete modelling of a limited number of flow paths. The channels are assumed to be one-dimensional and no mixing is assumed to occur between the channels. The transport in each channel is calculated individually and the total release rate is obtained by adding the release rate from all channels. Alternatively, the channels can be grouped in flow rate ranges and the release rate from each group is calculated and multiplied by the fraction of flow in that group.

The transport within an individual channel may be calculated with the advection-dispersion equation considering matrix diffusion and sorption, and radionuclide decay. The main difference from the modelling described in the previous section is that in the channeling model there is no mixing between channels and that the geometry for the matrix diffusion is different. Very little is known of the actual geometry of the channels. As for the advection-dispersion model it has been found that the effect of surface sorption and matrix diffusion is very much dependent on the specific surface of the channel. If the channels are delimited by the fracture walls a reasonable assumption is that the channels could be described as slits with a rectangular surface area. However, it has been shown [Rasmuson and Neretnieks, 1986b] that a slit formed channel can be approximated by a cylindrical channel with the same wetted surface area. For small penetration depths and for penetration depths much greater than the width of the channel, the diffusion from cylindrical and slit-formed channels will be similar. However, the assumption of cylindrical channels will overestimate the matrix diffusion somewhat for intermediate penetration depths.

Simplifications can be made in the channeling model, since the hydrodynamic dispersion within a single channel will be considerably smaller than the dispersive effect of the flow rate distribution, and can thus be neglected [Neretnieks, 1983]. In this case the concentration in the channel, c_f, is given by:

$$\frac{\partial c_f}{\partial t} + u\frac{\partial c_f}{\partial z} = \frac{2D_e}{\delta}\frac{\partial c_p}{\partial x}\bigg|_{x=0} - \lambda c_f \qquad \textbf{(3-13)}$$

and the concentration in the rock matrix, c_p, by:

$$\frac{\partial c_p}{\partial t} = D_a\frac{\partial^2 c_p}{\partial x^2} - \lambda c_p \qquad \textbf{(3-14)}$$

where:

δ is the channel aperture
D_a is the apparent diffusivity in the matrix ($D_a = D_e/\varepsilon_p R$)

The initial condition is zero concentration in both the channel and the matrix. The inlet boundary condition is a sudden step increase to c_0 in the fracture followed by a decrease due to radioactive decay and the outlet concentration is zero at infinite distance. With these initial and boundary conditions, the solution of the above equations becomes:

$$c = c_0 e^{-\lambda t}\ \mathrm{erfc}\left(\frac{D_e t_w}{\delta (D_a (t-t_w))^{1/2}}\right) \qquad \textbf{(3-15)}$$

The solution assumes an infinite matrix and is thus applicable when the radionuclide does not penetrate more than a fraction of the distance between two channels.

The water residence time is explicitly used in Equation 3-15. By using the relation:

t_w = channel volume/ flow rate in channel = $L \cdot W_{fr} \cdot \delta / Q$

we obtain:

$$c = c_0 e^{-\lambda t} \operatorname{erfc}\left(\frac{D_e L W_{fr}}{Q(D_a(t-t_w))^{1/2}} \right) \quad \textbf{(3-16)}$$

where:

L is the channel length
W_{fr} is the channel width
Q is the flow rate in the channel

It can thus be seen that for times considerably longer than the water residence times, $t >> t_w$, that the fracture aperture does not influence the results. This is of special interest for sorbing nuclides which are strongly retarded in relation to the water residence time. Then only times much larger than t_w are of interest.

Channel modelling in stream tubes.

In the channeling model the only assumption made regarding the geometrical position of the channels in the rock is that the individual channels will not intersect. The streamtube concept can therefore be applied by modeling a number of channels within each streamtube. These channels are then assumed to "follow" the extent of the streamtube in the rock and it will further imply that no channels will leave the streamtube. This is consistent with the assumption for the advection-dispersion model that there is no interaction between the different stream tubes.

For each streamtube the distribution of flow rates between the different channels must be given. Such a distribution will normally not be obtained from the large scale hydrology model producing the stream tubes, and must be obtained elsewhere.

A requirement for the application of the channeling model as stated in Equation 3-16 to a streamtube is that the cross-sectional area of the streamtube is large compared to the average spacing of the channels in order to include a reasonable amount of channels within each streamtube. If the number of channels is very limited the assumption that the hydrodynamic dispersion within a channel will be negligible compared to dispersive effect due to the distribution in flow rate between the different channels. However, the effect of channeling, even with only one channel per streamtube, can in principle be described by the advection-dispersion equation.

3.2.3 Network models

The Fickian type of dispersion used in the advection-dispersion model will give a spreading of a concentration pulse of the kind that can be expected when a frequent mixing of the flowpaths occurs. The channeling model does not take into account any mixing of the water between different flow paths in the rock. The spreading of a concentration pulse will in this case be a function of the spreading of the flow rates between different channels. These two approaches represent two extremes of possible

dispersion behavior. In a real situation the hydrodynamic dispersion may lie somewhere between these two extremes.

Theoretical investigations have been performed studying the statistical moments for the residence time distribution of a network of channels [Rasmuson, 1985]. These statistical moments have been used to determine a criterion for when the response of a system of flowpaths can be described by Fickian dispersion. For situations where the mixing is not frequent enough to justify the use of the Fickian dispersion assumed in the advection-dispersion model, a channel network model may be used.

The network models are presently used as research models and are not yet ready for large scale applications in safety analyses.

Overview of transport network models

Discrete fracture network models were originally developed for flow calculations [Robinson, 1984; Long et al., 1985; Dershowitz et al., 1985; Andersson and Dverstorp, 1987], but have more recently also been extended to include solute transport [Dverstorp, 1991; Cacas et al., 1990]. A network of fractures or channels is generated stochastically in a three dimensional space. The fractures are often modeled by simple geometrical structures such as discs or rectangles. The models need data such as fracture frequency, orientation, dimension and transmissivity. Channeling may be described by placing flow paths within the fracture planes. The transport within the individual network segments is usually described by the advection-dispersion model. However, the dispersion within an individual flow path is often considered to be of minor importance compared to the dispersion caused by variations between channels, and is therefore treated in a simplified way or even neglected. The effect of surface sorption can easily be included into fracture network models, but the inclusion of matrix diffusion is more complex, especially in large networks.

A three-dimensional channel network model has been developed by Moreno and Neretnieks [1991]. The approach used in this model is to independently generate a stochastic network of channels rather than to start with a simulation of the fractures. The channel network is visualized as a three dimensional rectangular grid of potential connections. At each intersection up to six channel segments can meet. It should be noted that the rectangular network does not reflect the real geometry of the network, e.g. different lengths of the channel segments can be simulated by modifying their conductance, or channel segments can be removed by assigning them an negligible conductance. Also variations in channel frequency and anisotropy can be simulated in a simplified manner.

The properties within an individual channel segment are assumed to be constant. The conductance is determined by the average transmissivity along the channel and the length of the channel. For the solute transport the volume of the channel and the flow-wetted surface are also needed. Hydrodynamic dispersion within individual channels is assumed to be negligible compared to the differences in residence time between channels. A full mixing is assumed to occur at the channel intersections.

The water flow rate within a channel segment is proportional to the pressure difference between the two connecting nodes. The pressure in the nodes of the network is calculated in analogy with Kirchoff's law for electrical resistors. The flow within each channel segment can easily be calculated knowing the pressure distribution.

The solute transport is simulated using a particle-tracking technique. For non-sorbing species the residence time in an individual channel is determined by the channel flow rate and the channel volume. The total residence time of a particle in the network is given by the sum of the residence times in every channel the particle has traversed. The residence time distribution is obtained by using a multitude of particles.

When hydrodynamic dispersion within a channel or matrix diffusion is considered, different particles in the same channel may have different residence times. The distribution in residence times is therefore expressed as a probability density function, which is derived from the outlet concentration resulting from a pulse injection into the channel. In the case of matrix diffusion the analytical solution of the channeling model is used, Equation 3-16. This is the only one of the mentioned network models which presently can handle matrix diffusion.

Applications to stream tubes

The channel network model has so far mostly been applied to cubical domains of the size of 20 x 20 x 20 nodes. Modelling has been for a parallel flow system and for a system with converging flow. In the parallel flow system a constant potential difference is assumed between the top and bottom surface of the cube, while no flow is assumed to occur through the sides. This corresponds to the transport in a stream tube. As long as the transversal spread of a tracers is so small that the no-flow boundaries at the sides will not affect the outlet concentration, the assumption of no interaction between the stream tubes can be used.

The effect of the boundaries will depend of the size of the tracer inlet, the dimensions of the cube and the variation of the channel conductance. Tests have been made with downward flow and a tracer inflow with a point source at the top of the cube. In the simulations the conductance of the channels was assumed to be log-normally distributed with a mean μ_0 and a standard deviation σ_c. In the case of a low variation of channel conductance ($\sigma_c = 0.2$) most of the tracer comes out at a limited area directly under the point of injection. For a large variation in conductance ($\sigma_c = 1.2$) a considerable spreading and many peaks in the outlet flow was found.

3.2.4 Comparison of the models

Three types of models have been described above:

- the advection-dispersion model
- the channeling model
- the channel network model

The first model is based on the continuum approach, i.e. an averaging of the transport properties over a larger volume is made. The rock in this volume is assumed to have the properties of a continuous medium. The different parts of the rock are modelled as two separate continua (the dual porosity approach), e.g. the fissures with flowing water and the microfissures of the matrix with stagnant water.

The second two models are based on the discrete modelling of individual flowpaths in the rock. The properties of these flowpaths are based on observations in the field. However, since the number of flowpaths may be very large and the properties of the flow paths may differ substantially, a statistical approach is generally needed. The main difference between the channeling model and the channel network model is the degree of connections between the flowpaths. In the channeling model no mixing between flowpaths is assumed, while in the channel network model mixing may occur.

Model properties and capabilities

The advection-dispersion model and the channeling model give very similar results when used to simulate the result of a tracer experiment with a non-sorbing tracer [Moreno et al., 1985]. The fitted breakthrough curve will be almost identical. However, important differences may appear when using the fitted parameters for predictions of other situations.

When the breakthrough curve is predicted for non-sorbing nuclides for the same migration distance, but with a different water velocity, the results are the same with the two models, if the dispersion coefficient is assumed to be proportional to the water velocity, as is usually done. However, if the migration distance is increased the channeling model predicts a greater dispersion than the advection-dispersion model using a constant dispersion coefficient. The early breakthrough predicted by the channeling model may be of importance for some radionuclides. The channelling model predicts a scale dependent dispersion coefficient, proportional to the distance. This can be "simulated" when using the advection-dispersion model by assuming a constant Peclet value when extrapolating the results of a tracer experiment to longer distances. In such a case the two models would give similar predictions. It should be noted that field observations indicate that the dispersion coefficient increases with observation distance [Neretnieks, 1985].

The dispersion behavior of the two models may differ if surface sorption is considered. In tracer experiments non-sorbing tracers are generally used. Residence times and Peclet values or σ for the channel aperture distribution may be derived from such experiments and the behavior of sorbing radionuclides are predicted by applying a surface sorption coefficient, K_a. In the channeling model it may be assumed that the flow is within parallel-walled channels with an aperture distribution $f(\delta)$. For laminar flow the flow rate will be proportional to the cube of the aperture. This will cause a very large portion of the total flow to go through the larger channels. The residence time for the water in the channel will be inversely proportional to the square of the aperture. However, the contact area between the flowing water and the solid will also depend on the channel aperture and thereby also the retardation factor, which is given as:

$$R_a = 1 + 2K_a/\delta \qquad \textbf{(3-17)}$$

For even rather low values of K_a, the term "1" in Equation 3-17 can be neglected and the retardation factor will be inversely proportional to the channel aperture. Thus, the larger channels will have high flow rates, short water residence times and relatively low retardation factors. For the smaller channels the effect is the opposite. This will lead to an increased spreading of the breakthrough curve.

In summary it can be stated that this "additional" spreading is due to the correlation between the specific surface (and thereby the retardation factor) and the water residence time. It has been suggested that this correlation could be derived from the assumption of flow in channels within parallel fractures determined by the hydraulic aperture using the cubic law. This may not be a completely realistic description of the flow. In reality the channels may have a varying aperture where the constrictions with small aperture will play an important role for the channel conductance and the parts with large aperture will determine the channel volume and thereby the contact area per unit volume of water. However, for the wide range of flow rates observed in nature, many orders of magnitude, it seems reasonable to assume some correlation between specific area and water residence time. However, this has not yet been determined experimentally.

In the advection-dispersion model there is no implicit relation between contact area between the rock and the flowing water and the water velocity, only a total contact area is given. Thus, the inclusion of surface sorption by a retardation factor will give an equal retardation of the early part of the breakthrough curve as for the late part.

If the effect of matrix diffusion is considered, a more pronounced difference in spreading appears between the channeling model and the advection-dispersion model when predicting the transport over longer distances. The reason is that the effective retardation due to the matrix diffusion and sorption will be time dependent in any given location. In the channels with short water residence time the amount that can diffuse into the matrix will be less than in the channels with long water residence time. The advection-dispersion model also assumes that a part of the radionuclides will travel faster, giving a shorter time for diffusion into the matrix. However, since the advection-dispersion model is based on the continuum approach an averaged concentration is used and it is implicitly assumed that all surface area is available for matrix diffusion, although the fast moving radionuclides are conceptually believed to be in a limited part of the stream tube with fast flow. If the available surface area was the same in all flowpaths in the streamtube regardless of the water velocity, the reduction in concentration by using an average value would compensate for the increased area. However, since it is reasonable to believe that there is a smaller contact area per volume of water in the parts with a fast water flow, the result will be an overestimation of the retarding effect of matrix diffusion in the fast pathways.

In the channel network model the dispersion will not only depend on the variation in flow rate in the different channel segments, but also on the connectivity at channel intersections. In each intersection there is a possibility to have connections between six channel segments. However, with an increasing standard deviation of conductance some of the segments at an intersection will have negligible conductance. Studies have shown that the connectivity of the network is strongly reduced when the standard deviation of conductance is increased [Moreno and Neretnieks, 1991]. For very high variations in the conductance of the channel segments, the flow situation will then be similar to that of the channeling model.

The discussion above shows the importance of determining the relation between the specific area, flow rate (or conductance) and water residence time (or channel volume). Simulations with the channeling model show the importance of the relation between specific area and water flow rate. Comparisons between the advection-dispersion model and the channeling model show that the choice of model is of great importance for predictions made for other situations. The predicted breakthrough curves for longer distances using the channeling model show a higher dispersion and an earlier arrival than those predicted by the advection-dispersion model. The same effect is also noticed when predicting the breakthrough for radionuclides with surface sorption and matrix diffusion. Simulations with the channeling network model show that the choice of relationship between channel volume and channel conductance is of great importance for the dispersion obtained for non-sorbing tracers, whereas it has no noticeable impact for sorbing tracers. This is expected also from the theory.

Computational considerations for transport models in stream tubes

The application of the advection-dispersion model with matrix diffusion to a stream tube requires only solutions in one dimension. With simple boundary conditions and constant parameters relatively simple analytical solutions can be used. The inclusion of chain decay will complicate the problem, but for example semi-analytical solution may be used, as in FARF31. In the case of varying parameters, when averages or effective values are deemed inappropriate, or more complex geometries for the matrix diffusion numerical solutions are needed, e.g. by using the computer code TRUCHN [Rasmuson et al., 1982]. Since discretization is only needed along the stream tube with a perpendicular component to describe the matrix diffusion the number of nodes needed will be relatively limited. However, the inclusion of chain decay may lead to numerical difficulties giving long computation times.

The channeling model is based on a simple closed form expression. However, for each stream tube several calculations are needed in order to take into consideration the distribution in flow rates between the classes of channels. In spite of this the computational effort needed is very small. At present only single radionuclide decay is included and not multiple chain decay. It is of course possible to use any advection-dispersion model solution, e.g. FARF31 to calculate the transport in the individual channels. Then also chain decay is automatically included.

The channel network model has large requirements on computer storage and computation times. So far grids of the size 20x20x20 have mostly been used. The actual physical dimension of such a grid will depend on the assumed channel spacing and channel lengths. The model is presently used as a research model and radioactive decay has only recently been included.

Final considerations for SKB 91

The above models, advection-dispersion, channeling and channel network, can be made to give similar residence time distributions for sorbing species for appropriate choices of parameter values. The key parameters are water flux, flow-wetted surface, and the parameter(s) which determine the dispersion. For non-sorbing species also the porosity

plays a role. In the advection-dispersion model the dispersion is described by the dispersion coefficient, in the channeling and the channel network models by the flow rate distribution and aperture distribution of the channels.

In SKB 91 the advection-dispersion model was used. The flux was derived from hydrology calculations, the flow-wetted surface from estimates based on field observations. The dispersion coefficient is derived from field observations and is taken to increase with stream tube length, i.e. a constant Peclet number is used.

4 DATA FOR TRANSPORT MODELS

4.1 Advective flux and groundwater travel time in stream tubes

In SKB 91 the transport pathways from the repository are described by 88 stream tubes originating from selected positions distributed over the repository, see Section 3.1.2. The geohydrological model used in SKB 91, HYDRASTAR [Norman, 1991] provides the advective fluxes at the repository level and the groundwater travel times for the individual stream tubes. The advective fluxes are used by the near field model and the groundwater travel times by the radionuclide transport model FARF31. The groundwater residence time distribution was calculated assuming a flow porosity of 10^{-4} throughout the rock.

In order to obtain statistics of the advective fluxes and groundwater travel times have a series of realizations been performed of the conductivity field based on measured hydraulic conductivity data. For the reference case, 500 realizations have been performed [Jansson, 1992] giving a median advective flux of 10^{-3} m^3/m^2,a and a median groundwater travel time of 700 years for all 500·88 stream tubes. There are large variations both in the results for different stream tubes in a single realization as well as in the results for a given stream tube between different realizations.

The median of the groundwater travel time in the 88 stream tubes varied between roughly 6 years and 10000 years between the different realizations. It should be noted that stream tubes with a water residence time longer than 10000 years have been assigned a value of 10000 years. The results from the 500 realizations show that around 44% of all 44000 stream tubes have groundwater travel times longer than 10000 years. The remaining 56% of the stream tubes are in a separate group with groundwater travel times in the range 10 to 1000 years. This can be explained by the presence of several separate discharge areas, one in the leveled area traversed by the Imundbo zone, one or several discharge areas further downstream, and a small discharge area west of the repository.

A small number of stream tubes will have short groundwater travel times. In 50% of the realizations did the 4 fastest stream tubes have a groundwater travel time less than 40 years, (i.e. the median of the 5-percentile for the groundwater travel time for each of the 500 realizations was 40 years). The short travel times were almost exclusively for the stream tubes originating from positions at the NE corner of the repository close to fracture zone 1.

The median in advective flux for all stream tubes varied between roughly 10^{-4} and 10^{-2} $m^3/(m^2,a)$ between the different realizations. There was also considerable variation in flux between different stream tubes within a single realization. In 50% of the realizations did the 4 stream tubes with the highest flux have a flux greater than $8 \cdot 10^{-3}$ $m^3/(m^2,a)$, i.e. the median of the 95-percentile for each of the 500 realizations was $8 \cdot 10^{-3}$ $m^3/(m^2,a)$.

The correlation between groundwater travel time and fluxes at repository level was found to be weak. The correlation coefficient was around -0.3 for the logarithmical values.

4.2 Dispersion

Measurements of dispersion.

The dispersion coefficient, D_L, may be determined from the spread of a tracer pulse in a tracer experiment. A major problem is that such experiments have been performed only over relatively short distances, typically 10 - 50 meters. Compilations of available data indicate that the dispersion length increase with the migration distance [Neretnieks, 1985]. However, definite conclusions are difficult to make due to the different methods used in the experiments and due to varying quality of the data. Thus, the extrapolation of data from tracer experiments is uncertain.

The spreading of the concentration pulse due to dispersion can in some cases be overshadowed by other effects such as matrix diffusion. The matrix diffusion may dominate the spreading of the pulse if the contact times are long [Neretnieks, 1983].

The dispersion coefficient is often assumed to be proportional to the migration length and to the water velocity - the Peclet value is constant ($Pe = u \cdot L/D_L$). This is in principle contradictory to the assumptions in the advection-dispersion model where the dispersion coefficient is implicitly assumed to be independent of the accumulated distance traveled. This contradiction is circumvented by assigning a dispersion coefficient value which gives the "correct" spreading of the pulse at the outlet end. In the case when applying the advection-dispersion model to the stream tube concept the water flux may also vary along the stream tube. A method to derive an effective Peclet number in a strongly varying velocity field by adding the variances in residence time of flow sections coupled in series has been developed [Neretnieks and Rasmuson, 1984]. Although this method is based on assumptions valid for cases with small dispersion, it has been used with large dispersion and large velocity variations with small errors [Rasmuson and Neretnieks, 1986a]. However, in a more recent study it has been found that the method of adding variance may lead to too high dispersion in cases with very low water velocities in parts of the stream tube, this results in a too early arrival of the radionuclides [Bengtsson et al., 1991].

When pure channeling occurs the dispersion length ($\alpha = D_L/u$) increases with migration distance. In the channeling model, the dispersion is not given as a direct input variable, but will be determined by the distribution of flow rate between the different flow paths.

In the application of the advection-dispersion model to the repository, described in Section 3.2, the repository will be divided into roughly a hundred stream tubes. Each stream tube would thus have an initial cross-sectional area of 100 by 100 meters and would describe the transport from roughly 50 waste canisters. Such relatively large stream tubes can contain a large number of water bearing channels (typically a hundred to several hundred), and thus the dispersion value chosen for the stream tube should simulate the dispersion due to velocity distributions between these channels. However, this velocity distribution is not given by the results of the continuum approach hydrology model used to derive the stream tubes, but must be obtained elsewhere.

In the channeling model the standard deviation of conductivities or flow rates among the channels is obtained by fitting to field data on dispersion in the same manner as when the dispersion coefficient is obtained in the advection-dispersion model. It is in fact possible

to obtain a simple expression relating the Peclet number to the standard deviation of conductances [Neretnieks, 1983; Moreno et al., 1985].

Dispersion data

Table 4-1 lists the evaluated dispersion lengths from some tracer experiments in fractured crystalline rock [Neretnieks, 1985]. The table also gives the Peclet value with and without matrix diffusion. In the experiment from the Finnsjö site the condition of the fracture surface was not known, but a regression analysis indicated that the matrix diffusivity was much higher than in intact granite. In this case matrix diffusion would account for most of the pulse spreading.

In Figure 4-1 the dispersion length is plotted as a function of migration length for the experiments listed in Table 4-1. This compilation of data must be considered approximate since different methods have been used to determine the dispersion coefficient.

Computer simulations of transport in fissured media have also been used to derive dispersion data [Dverstorp, 1991; Moreno and Neretnieks, 1991]. In realizations with large standard deviations in flow path conductance frequently very low Peclet numbers have been obtained, i.e. less than 1. Flow paths with very high dispersion values (Pe < 1 - 4) were also found in the Stripa 3D experiments [Abelin et al., 1987]. However, an exact evaluation of these low Peclet number was not possible with the model used.

Based on the data from the experiments listed in Table 4-1 and the occurrence of flow paths with very low Peclet number a wide range (0.2 - 20) is recommended for the transport calculations. This range covers most of the observed and simulated data. A central value of 2 has been chosen, see Table 4-3.

4.3 Flow porosity and flow-wetted surface

The contact area between the rock and the flowing water - the flow-wetted surface - is of great importance for the retardation by surface sorption and matrix diffusion. Very little is known of the flow-wetted surface present in fractured rock and no established procedures are available to measure the specific surface in a rock.

When the advection-dispersion model is used the flow-wetted area can be described by the specific surface parameter. This can be given as specific surface per unit volume of flowing water, a, or specific surface per unit volume rock, a'. In view of the lack of experimental data the specific surface is often estimated from assumptions concerning the frequency and geometry of the fissures in the rock.

It may be noted that flow porosity is poorly known, but on the other hand does not much influence the velocities of sorbing nuclides. The spacing between conductive fissures, S, is more amenable to measurements which can be made in bore holes. A fissure spacing of 5 meters and a fissure aperture of 0.1 mm would in the case of parallel fully open fissures give a flow porosity of $2 \cdot 10^{-5}$. The specific surface per unit volume of flowing water would for the same case be 20 000 m^2/m^3 and the specific area per unit volume of rock 0.4 m^2/m^3.

The flow porosity was evaluated from the results of the 3D migration experiment in the Stripa mine [Abelin et al., 1987]. The obtained values varied between $2 \cdot 10^{-5}$ and $7 \cdot 10^{-5}$ for the rock far from the drift, while the rock in the 10 meters nearest to the rock was found to have a porosity of $1.6 \cdot 10^{-4}$. However, there are large uncertainties in the determination of a large scale average flow porosity experimentally.

For the transport calculations a range of 10^{-5} to 10^{-3} is recommended with a central value of 10^{-4}, see Table 4-3.

Tracer experiments in Stripa have also been used to derive values of the specific surface per unit volume of rock. The specific 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. Matrix porosity and diffusivity data for the model predictions were taken from laboratory diffusion measurements [Abelin et al., 1987]. The specific area per unit volume of rock was estimated to be between 0.2 and 2 and possibly up to 20 m^2/m^3. The uncertainty in these values are due both to the fact that parameters used in the model prediction are taken from laboratory measurements on samples of rock not in direct contact with a fracture with flowing water and to the fact that it is not certain that all of the non recovered tracer has diffused into the rock matrix. Other possible sources for the limited recovery has been proposed, e.g. diffusion into stagnant volumes of water or the disappearance through other flow paths not leading to the sampling point.

In the channeling model and the channel network model the flow-wetted area is given by specifying a channel width. Estimations of channel widths have been made from observations in tunnels and drifts. From observations in the Kymmen tunnel it was found that 99.7% of the channels were less than 0.1 meter wide [Palmqvist and Lindström, 1991]. In observations of the tunnels and drifts of the Swedish final repository for radioactive 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]. In the channeling experiment performed at Stripa the channels widths were in the order of decimeters or less [Abelin et al., 1990].

The flow-wetted surface has also been estimated from field observations of channels [Moreno and Neretnieks, 1991]. A cubic grid of channels is assumed with a channel length between 1.2 and 10.2 meters, derived from data for different sites in Sweden. With a channel width of 0.1 meters this yields a flow-wetted surface per unit volume of rock of 0.006 - 0.4 m^2/m^3.

Due to the large uncertainties in the data a wide range is recommended for the transport calculations (0.01 - 0.5 m^2/m^3). A specific surface per unit volume of rock of 0.1 m^2/m^3 has been chosen as central value, see Table 4-3.

Within the SKB 91 project an alternative model based on the discrete fracture network concept has been used to estimate the hydrological and transport properties of the rock at the Finnsjön site [*Geier et al., 1992*]. The purpose has been to evaluate the information obtained from packer tests; to determine whether the rock in a practical sense behaves as a stochastic continuum; and to estimate reasonable values for the transport parameters.

The discrete fracture network model is based on a statistical description of the geometric and hydraulic properties of the rock. The required input data are statistical distributions of fracture properties such as location, size, orientation, transmissivity, and intensity (i.e. total fracture area per unit volume of rock). These data are used to simulate different fracture populations. The flow paths are assumed to result from an interconnected network of fractures.

Analyses of geometric and hydrologic data, e.g. outcrop maps, scanline surveys, core data and steady state packer tests provide the required statistics. The various procedures for deriving these statistics are largely independent and thus some aspects of the model can be partly validated by comparing the results of transient constant-pressure packer test with the predictions made by the model.

The hydrological behavior of the fracture system is modelled explicitly for scales up to the block size used in the three-dimensional stochastic continuum models (HYDRASTAR: 36x36x36 meters). The large scale behavior is described in terms of spatial correlation of block-scale properties. Each fracture is assigned an average transmissivity and storativity, dependent on the stress field.

With the discrete fracture network model the flow porosity and the flow-wetted surface have been estimated based on block-scale simulations. Additionally, the estimations require assumptions concerning the relationships between subfracture transmissivity, flow aperture, and wetted surface per unit area of the fracture plane.

Estimations have been made of the flux-weighted averages of the flow porosity and the flow-wetted surface for use in FARF31 as well as the values for specific ranges of element flux, given as histograms. The estimates were produced for a base case and for a case when all fractures with a transmissivity higher than a given value were assumed to be breccia-filled. In the breccia-filled fractures the available surface area may be orders of magnitude larger than in coated fractures. The estimates were produced for averaging volumes on scales ranging from 20 to 40 meters. Estimates of the flow porosity varied between $3 \cdot 10^{-6}$ and $4 \cdot 10^{-5}$ for the base case. For the breccia case a flow porosity around $5 \cdot 10^{-6}$ was obtained. The flux-averaged flow porosity was around $5 \cdot 10^{-6}$ for the base case. The flow-wetted surface obtained varied between 0.0017 and 0.016 m^2/m^3 rock for the base case. For the breccia case the flow-wetted surface was roughly an order of magnitude higher. The flux-averaged flow-wetted surface was around 0.002 m^2/m^3 of rock for the base case. No correlation was found between the estimated values of flow-wetted surface and flow porosity.

The estimates of flow-wetted surface obtained with the discrete fracture model are lower than the values obtained from experiments and in the lower range of the values obtained from estimates based on channel lengths, see Table 4-2. The results obtained with the discrete fracture model are associated with large uncertainties both due to the simplified relationships assumed between hydraulic aperture, void aperture, and fracture specific surface, as well as due to the limited data available to characterize the rock. Especially, information to characterize the fractures and the possibility of channeling in fractures are missing.

4.4 Matrix diffusivity and porosity

The matrix diffusivity of crystalline rock has been extensively measured in the laboratory. A large number of measurements has been performed on rock samples from the Finnsjö site using non-sorbing tracers. Also measurements of the porosity has been performed on the Finnsjö rock. Comparisons between field scale experiments in the Stripa mine [Birgersson and Neretnieks, 1990] and laboratory experiments [Skagius, 1986] show that results from laboratory experiments are representative for field conditions. A compilation of rock matrix diffusivity and porosity data has been performed within the SKB 91 project [Brandberg and Skagius, 1991]. The values proposed in this report for the matrix of the rock at Finnsjön are:

Effective matrix diffusivity, $D_e = 1 \cdot 10^{-13}$ m^2/s
Diffusion porosity, $\varepsilon_p = 0.5\%$

4.5 Sorption coefficients

The different interaction mechanisms between a radionuclide in the solute and on the solid surfaces are generally modelled as a linear equilibrium sorption process where all the effects are added into an effective sorption coefficient or K_d-value. The K_d-values are based on empirical data measured for conditions similar (or as similar as possible) to the conditions prevailing in the rock. Within the SKB 91 project a compilation of K_d-values for the different radionuclides has been performed [Allard et al., 1991].

Table 4-1 Dispersion lengths and Peclet numbers evaluated from tracer experiments.

Experiments	Migration distance	Dispersion length	Peclet number		Fissure aperture
	m	m	(a)	(b)	mm
Laboratory experiment with natural fissure [Neretnieks et al., 1982]	0.3	0.025	12	12	0.18
Laboratory experiment with natural fissure [Moreno et al., 1985]	0.19 0.27	0.005 0.011	38 25	38 25	0.15 0.14
Stripa natural fissure. Two different channels. [Abelin et al., 1983]	4.5 4.5	2.0 0.62	2.2 7.3	– –	0.11 0.14
Studsvik site 2 [Landström et al., 1982]	14.6	–	–	37	–
Finnsjön site [Moreno et al., 1983]	30	{0.35 5	87	5	{0.47 0.98
Studsvik site 1 [Landström et al., 1978]	22 51	6.1 7.7	– –	3.6 6.6	– –
French site [Lallemand-Barrès et al., 1978]	11.8	0.8	–	14.8	–
U.S. site [Webster et al., 1970]	538	134	–	4.0	–

a) Peclet number evaluated without accounting for matrix diffusion
b) Peclet number evaluated accounting for matrix diffusion

Table 4-2 Compilation of estimates of flow-wetted area

Experiment	Flow-wetted area (m^2/m^3 rock)
Stripa 3D [Abelin et al., 1987]	0.2 - 2.7 0.5 - 27
Stripa SCV [Birgersson et al., 1992]	5 - 24
Estimated channel lengths [Moreno and Neretnieks, 1991]	0.006 - 0.4
Discrete fracture modelling [Geier et al., 1992]	0.0017 - 0.016

Table 4-3 Example of parameter values for the transport calculations. See text for discussion of chosen values.

Parameter	Notation	Central value	Range	Unit
Water flux at repository level	u_0	1	0.1 - 10	l/m^2,a
Groundwater travel time	t_w	700	10 - 10000	a
Peclet number	Pe	2	0.2 - 20	-
Specific surface per unit volume of rock	a_R	0.1	0.01 - 0.5	m^2/m^3
Flow porosity	ε_f	10^{-4}	10^{-5} - 10^{-3}	-
Effective matrix diffusivity	D_e	$1 \cdot 10^{-13}$		m^2/s
Diffusion porosity	ε_p	0.005		-

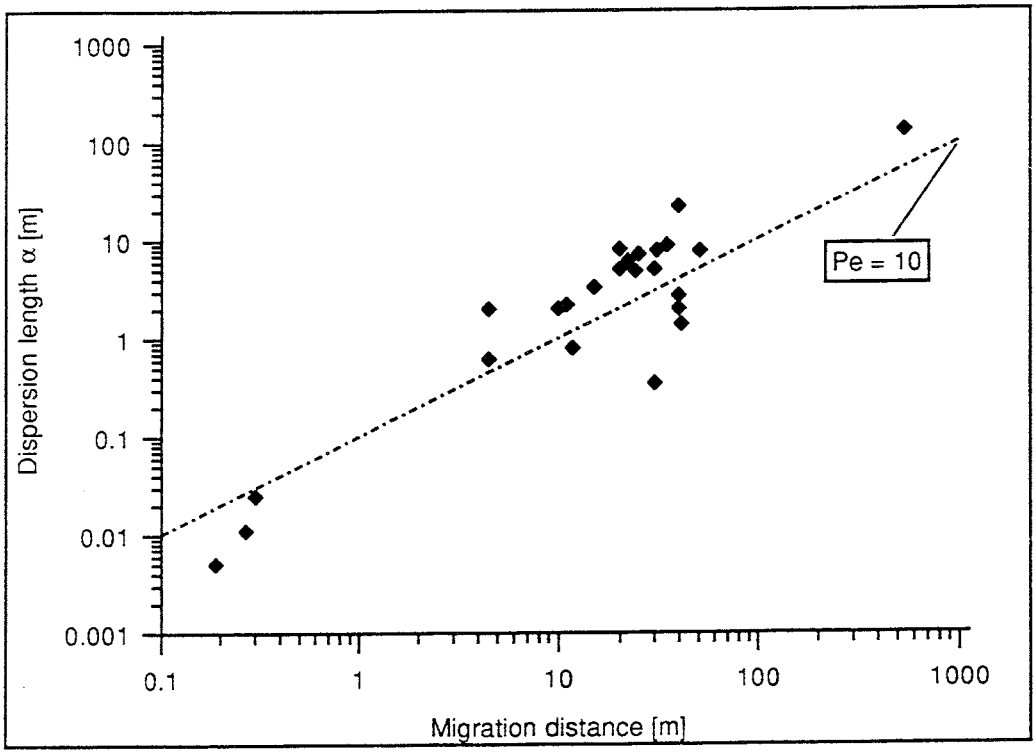

Figure 4-1 Experimentally determined dispersion lengths from Table 4-1, as a function of migration distance, [Neretnieks, 1985].

5 SUMMARY AND DISCUSSION

This report provides a conceptual description of the radionuclide transport in crystalline rock as well as a description of the modelling approach for far field transport used within the SKB 91 project. Furthermore, the data needed for the transport models are discussed and recommended ranges and central values are given.

In the SKB 91 project a site-specific performance assessments is performed for a KBS-3 type repository for spent fuel in crystalline rock. The main objective is to visualize and quantify the effect of different geological parameters affecting the long-term safety. In the KBS-3 concept the repository for spent nuclear fuel will be located deep in the crystalline bedrock and the isolation of the waste will be achieved by a combination of engineered and natural barriers. If the copper canisters containing the spent fuel fail, radionuclides will be released through the surrounding backfill material and may be transported by the groundwater in the waterbearing fractures in the rock. The main process for transport of radionuclides is with the flowing groundwater. Variations in flow between different flow paths will cause a spreading of the radionuclides - dispersion, which influences the breakthrough time. Most radionuclides will interact with the rock and will thereby be retarded in relation to the velocity of the water. This may be due to sorption on the fracture surface - surface sorption - or due to diffusion into the porous rock matrix and sorption on the large inner surfaces of the rock matrix.

Several types of models have been developed for quantifying the radionuclide transport in the far field. In this report a comparison is made of the properties and capabilities of the advection-dispersion model, the channeling model and the channel network model. The first model is based on the continuum approach, while the other two are based on a discrete modelling of individual flowpaths. All models give similar results when used to simulate the results of a tracer experiment. However, important differences may appear when using the fitted parameters for predictions of other situations. Prediction of breakthrough curves for longer distances with the channeling model gives an earlier arrival than those predicted with the advection-dispersion model.

The modelling of the far field radionuclide transport within the SKB 91 project is made with an advection-dispersion model based on the stream tube concept. A stream tube is an imaginary tube defined as a volume enclosed by a set of streamlines generated by a groundwater flow model. Since no transport of radionuclides is assumed to occur between different stream tubes, the transport within each stream tube can be modelled independently. The stream tube concept greatly facilitates the radionuclide transport modelling. Instead of having to model the radionuclide transport in three dimensions with the complex three-dimensional flow field obtained in the hydrology calculations, a set of one-dimensional calculations is performed. In the present calculations the repository is divided into 88 parts each encompassed by a stream tube. Each stream tube covers 50 to 60 spent fuel canisters. The transport of radionuclides along each stream tube is calculated with a dual-porosity continuum model based on the advection-dispersion equation. The model takes into account matrix diffusion, sorption in the rock matrix and radioactive chain decay. The model is based on flux-averaged quantities of concentration, water velocity, dispersivity and the exchange rate between the flowing water and the pores of the rock matrix.

The key parameters are the water flux, the contact area between the flowing water and the rock (*flow-wetted surface)*, and the dispersion coefficient. The matrix diffusion and sorption is determined by the effective diffusivity of the rock matrix and the sorption coefficient of the radionuclides. For non-sorbing species also the flow porosity plays a role. For the radionuclide transport calculations in SKB 91 the distribution of advective fluxes and groundwater travel times in the stream tubes are derived from series of realizations performed with the geohydrological model. The flow porosity and flow-wetted surface is estimated based on field observations. These parameters are associated with large uncertainties due to difficulties in performing measurements in undisturbed rock and interpreting the results. Reported values vary within a wide range. The dispersion coefficient is derived from values obtained in field experiments and is taken to increase with stream tube length, i.e. a constant Peclet value is used.

NOTATION

a_R	Specific surface per unit volume of rock	m^2/m^3
a_W	Specific surface per unit volume of flowing water	m^2/m^3
c	Radionuclide concentration in the pore water	Bq/m^3
c_f	Concentration in the channel	Bq/m^3
c_i	Concentration of nuclide *i* in the flowing water	Bq/m^3
$c_{p,i}$	Concentration nuclide *i* in the rock matrix pores	Bq/m^3
D_a	Apparent diffusivity in the matrix	m^2/s
D_e	Effective diffusivity in the rock matrix	m^2/s
D_L	Dispersivity	m^2/s
F_{in}	Input flux of radionuclide	Bq/s
F_{out}	Output flux of radionuclide	Bq/s
K_a	Surface sorption coefficient	m^3/m^2
K_d	Sorption coefficient	m^3/kg
L	Channel length	m
Pe	Peclet number	-
Q	Flow rate in the channel	m^3/s
Q_{tube}	Flow rate in stream tube	m^3/s
R	Retardation factor	-
R_a	surface retardation factor	-
R_i	Matrix retardation factor	-
S	fissure spacing	m
t	Time	s
t_w	Water residence time	s
u	Water velocity	m/s
u_0	Water flux (Darcy velocity)	m^3/m^2,s
W_{fr}	Channel width	m
x	Distance into the matrix	m
x_0	Maximum penetration depth in matrix	m
z	Distance in the flow direction	m
Z	Migration distance	m

α	Dispersion length	m
δ	Channel aperture	m
ε_f	Flow porosity	-
ε_p	Diffusion porosity of the matrix	-
λ_i	Radioactive decay constant for nuclide *i*	1/s
μ_0	Mean of channel conductance	-
ρ	Solid density of the rock	kg/m^3
σ_c	Standard deviation of channel conductance	-
ζ	Distance in flow direction expressed in terms of groundwater travel time	s

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