Working Report 2007-24

A Concept for Radionuclide Transport Modelling

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ABSTRACT

This report drafts a modelling methodology that can be applied to assess transport and retention properties along flow paths in fractured rock. Transport properties are assessed for the main geosphere retention processes: matrix diffusion and sorption. Data extracted from the flow model is used to characterise release paths and to derive appropriate geosphere performance measures that can be applied in the radionuclide transport calculations, performance assessment and safety case.

The proposed transport concept is based on application of the site scale DFN model. It is able to take into account heterogeneity in all scales. Computational feasibility can be ensured by focusing the detailed scale fracturing only to the regions of the model that have active flow paths or that are of special interest. The present transport concept takes advantage of the one dimensional nature of the solute transport through the fractured rock. In practice, this means that the transport channels are identified by particle tracking using the simulated DFN flow field.

Enhancements of the present approach compared to the previous analyses are, for example: site evolution is taken into account in the flow conditions, heterogeneity of the fractured rock is taken into account by explicitly including small scale fracturing into the model where it is appropriate, heterogeneity of the rock mass and geological materials is taken into account by taking advantage of the generalised retention models and varying sorption properties, in space or in time, can be taken into account.

Transport and retention simulations have important interfaces with DFN flow modelling, geology, geochemistry, biosphere modelling and performance assessment. DFN flow model has a central role in defining the flow characteristics, geology describes and parameterise the generalised retention models (immobile zones), geochemistry provide sorption data that are connected with the retention models and biosphere modelling provides the upper model boundary of the geosphere transport and retention model. Finally, performance assessment defines calculation scenarios and performance measures for the geosphere transport paths.

Keywords: Groundwater flow, transport of solutes, performance assessment, retention

Konsepti radionuklidien kulkeutumismallinnukselle

TIIVISTELMÄ

Tässä raportissa kuvataan laskenta- ja simulointimenetelmät, joita voidaan käyttää rakoilleessa kallioperässä olevien virtausreittien kulkeutumisominaisuuksien arviointiin. Kulkeutumisominaisuuksia arvioidaan ottamalla huomioon pääasialliset kallioperässä vaikuttavat pidättymisprosessit: matriisi diffuusio ja sorptio. Virtausreittien ominaisuudet selvitetään pohjavesivirtausmallinnuksen avulla. Virtausmallista johdetaan sopivat suureet, joilla voi mitata kallioperän kykyä toimia radionuklideja pidättävänä esteenä. Kallioperän kulkeutumisominaisuuksia kuvaavia suureita voidaan käyttää hyväksi radionuklidien kulkeutumissimuloinneissa, loppusijoitustilan toimintakyky-analyysissä ja safety case –analyysissä.

Esitetty kulkeutumiskonsepti perustuu tutkimuspaikan mittakaavan rakoverkkomalliin (DFN-malli). DFN-malli on valittu virtausmalliksi, koska se pystyy ottamaan huomioon kallioperän heterogeenisuuden eri mittakaavoissa. Tutkimuspaikan mittakaavan DFN-mallin laskennallinen toteutettavuus voidaan varmistaa kohdistamalla pienen mittakaavan rakoilu alueille, joilla on aktiivisia virtausreittejä tai jotka ovat muuten erityisen mielenkiintoisia. Sovellettava kulkeutumiskonsepti käyttää hyväksi rakoilleelle kalliolle havaittua aineiden kulkeutumisen yksiulotteista luonnetta. Käytännössä tämä tarkoittaa sitä, että kulkeutumiskanavat selvitetään seuraamalla virtaviivoja paikkakohtaisessa DFN-mallissa (particle tracking).

Esitetty kulkeutumiskonsepti tarjoaa parannuksia aiempiin analyyseihin verrattuna, esimerkiksi: tutkimuspaikan aikakehityksen vaikutukset virtauskenttään ja kulkeutumis-ominaisuuksiin voidaan ottaa huomioon, kallioperän heterogeenisuus on otettu suoraan rakoilun kuvauksessa huomioon, kalliomatriisin ja geologisten materiaalien hetero-geenisuus on otettu huomioon erilaisilla pidättymismalleilla ja ajallisesti tai paikallisesti muuttuvilla sorptio-ominaisuuksilla.

Kulkeutumisominaisuuksien arviointi perustuu simulointiin, joka on läheisessä ja tärkeässä vuorovaikutuksessa DFN-virtausmallinnuksen, geologian, geokemian, biosfääri mallinnuksen ja loppusijoitustilan toimintakykyanalyysin kanssa. DFN-virtausmallilla on kulkeutumiskonseptissa virtausominaisuuksien kuvaamisessa keskeinen osa, geologia antaa kuvauksen ja määrittelee pidättymismallit (immobiili huokoistilavuus), geokemiasta saadaan pidättymismalleihin liittyvät sorptio-ominaisuudet ja biosfääri mallinnus toimii kallioperän kulkeutumismallin yläreunana. Kulkeutumisominaisuudet selvitetään laskenta- ja simulointiskenaarioille, jotka määritellään osana loppusijoitustilan toimintakykyanalyysia.

Avainsanat: Pohjavesivirtaus, aineiden kulkeutuminen, pidättyminen

TABLE OF CONTENT

1 INTRODUCTION

Posiva's safety case is based on a portfolio composed of ten main reports. Radionuclide transport calculation is part of the analysis of the radiation safety. Radionuclide transport simulation is based on the site specific assessment of the potential release paths and estimated flow, transport and retention properties along the release paths. This requires models that are able to cover long periods of time and assess consequences of the expected evolution of the repository.

The main objective of this report is to draft a modelling methodology that can be applied to assess transport and retention properties along flow paths in fractured rock. Simulation of the transport and retention properties integrates data from many different sources and disciplines. Therefore, it is likely that the concept develops during the course of the site modelling and interim performance assessments. It is possible that the present concept will be updated in the future when practical experience on the data collection, simulations and model interfaces is available.

Transport properties are assessed for the main geosphere retention processes: matrix diffusion and sorption. The goal is to identify properties of the flow field that are important for the geosphere retention. Information extracted from the flow model is used to characterise release paths and to derive appropriate geosphere performance measures that can be applied in the radionuclide transport calculations, performance assessment and safety case.

Other transport related processes, like precipitation and dissolution, colloid-facilitated transport and gas-mediated transport, are discussed in conjunction with the assessment of the radionuclide transport as it is specified in the safety case plan (Vieno and Ikonen, 2005).

Flow modelling techniques are not a subject of this report and they are not discussed any further than is needed for understanding the assessment of the transport and retention properties.

2 FLOW IN FRACTURED ROCK

Transport and retention properties in the fractured rock are dominated by the typical features of the flow. This section gives a short summary of the dominant features of the groundwater flow in fractured rock that is of interest for the transport concept.

The main characteristics of groundwater flow through fractured rock are mainly determined by structure of the rock. Great heterogeneity in the local permeability and, correspondingly, large variability of the local flow rates are typical for the fractured rock. This leads to behaviour of the flow that can be described by three main properties: fractures are the main conduits (dual porosity of the fractured rock), flow takes place along distinct flow paths and the flow is channelized. Separation of the distinct flow paths from the overall channelling is not always necessary. In the present context, this separation is supported by the conceptualisation and nature of the flow problem. Channelling in the large scale (distinct flow paths) comes from the properties of the fracture network. In the small scale channelling is governed by the heterogeneity inside the fractures. The possibilities to collect information on the properties of the fracture network are much better than the properties to collect data on the individual fractures. This means that the treatment of the heterogeneity inside the fractures is usually based on the generic models and data, but the fracture network is more based on the measured data. This supports the applied separation to distinct flow paths and channelling.

2.1 Dual porosity

Fractured rocks are composed of porous but, in practice, impermeable rock matrix and water conducting fractures. The groundwater flow takes place dominantly through the fractures. Rock between fractures, the rock matrix, is porous and saturated by the water but it does not participate to the process of the groundwater flow. This means that fractures or the network of fractures are the main conduits of the groundwater flow. Fracture network is also the main transport pathway for the possible contaminants of the groundwater. It provides the inflow paths for the leaking groundwater during the construction and operational phase of the deep underground repository. Release paths from the possibly leaking disposal canisters to the biosphere go along the fracture network.

2.2 Distinct flow paths

The main characteristic of the fractured rock is the great heterogeneity in different scales. The heterogeneity is also a distinctive feature of the hydraulic properties of the fractured rock. Individual fractures and fracture zones can provide well conducting connections so that a few hydraulic features may dominate the overall flow conditions. In other words, the heterogeneous structure of the fractured rock leads to preferential flow paths that will govern both flow and transport properties through the rock mass.

Throughout the different scales fractures have a significant effect on flow and transport processes. There are indications that properties of the fractured rock cannot be homogenized in any scale. Instead, observations indicate that the fractured rock follows a scaling behaviour that does not exhibit any characteristic length scale (Berkowitz, 2002). However, the scaling behaviour is not the only feature of the fractured rock that causes channelling. The flow and transport behaviour is also governed by the fracture conductivities. Even a (geometrically) well-connected network can exhibit sparse preferential flow paths, if the distribution of fracture conductivities is sufficiently broad (Berkowitz, 2002).

Many in-situ tracer experiments have been carried out in the fractured rock during recent years. These tests indicate that tracer transport cannot be described accurately without considering distinct flow paths. Tracer experiments usually show fast initial arrival times, more than one peak in the breakthrough curves, and/or long tails and strong dependence of the transport characteristics on the scale (Becker and Shapiro, 2000; Nordqvist et al., 1996; Tsang et al., 1991). Modelling has shown that the preferential flow and transport paths run over long distances and reduce mixing in the tracer plume, especially in case of high transmissivity variance (Nordqvist et al., 1996). It also appears that the retention properties depend even more on the description of the preferential flow paths than the transport itself (cf. Section 3.2).

2.3 Channelized flow

Channelling has proven to be true and important process in the groundwater flow that has been addressed in many experiments and modelling exercises. It has also been found that 90% of fluid flow can occur through 5-20% of the fracture plane (Rasmuson and Neretnieks, 1986) and many field experiments indicate that only a limited part of the volume within the fractures, even less than 10%, is open to fluid flow and solute transport (Nordqvist et al., 1996).

In practice, it is very difficult to collect site specific quantitative data on the channelling. Modelling is usually based on the prescribed degree of channelling or generic models of the fracture heterogeneity and correlation lengths of the local transmissivity that appears to be reasonable.

3 SOLUTE TRANSPORT

This section discusses solute retention by matrix diffusion and sorption. The approach is to consider a small scale building block of the retention model, a streamtube that is composed of a bunch of streamlines. The size of streamtube is selected so that the molecular diffusion keeps solute concentration well mixed across the streamtube. In practice, this would mean that all particles in the streamtube have the same advective residence time, i.e. all particles undergo the same flow field when they pass through the streamtube. Streamtubes can be envisaged as individual, well mixed, transport channels in the context of the flow distribution in fractured rock. The approach applied in this section requires that the streamtube is simply connected and it is not branching. This is not a strict restriction, because in many cases branching streamtubes can be divided to smaller streamtubes that are not branching.

The main solute transport process is advection along with the groundwater flow. Basically, advection is controlled by the flow porosity and gradient of the hydraulic head. In the case of the fractured rock flow porosity is created by the aperture distribution along the flow path. Flow paths may involve different types of fractures and fairly large uncertainties are connected with the corresponding aperture distribution. This implies that the actual flow porosity experienced by the migrating solute could be quite uncertain.

The geosphere retention may have a significant influence on the solute transport through the bedrock. In many cases, due to the retention, solute residence times are much longer than the advective water residence times. It is possible that retention dominates the solute residence times so strongly that the influence of the advection is negligible.

The studied system of the streamtube next to the immobile pore space is illustrated *Figure 1*. Streamtubes lie on the fracture planes and they are connected to the immobile pore space that is, for example, in the rock matrix next to the fracture plane.

The main retention processes discussed in the present report are sorption and matrix diffusion. Retention processes are discussed by starting from a case of a single heterogeneous immobile zone in Section 3.1. A method to deal with the heterogeneity along the flow path is discussed in the Section 3.2 and the pattern of the heterogeneity is extended to several parallel immobile zones in Section 3.3. Assessment of the transport properties requires detailed description of the flow field. Section 3.5 discusses the required resolution of the flow field.

3.1 Matrix diffusion to one immobile zone

First, we consider advection-sorption-matrix diffusion equation in a case of one immobile zone along the flow path. The solute mass flux is studied over a small control volume as shown in the *Figure 1*. The streamtube that carries a fixed flow rate (denoted here by Q [L^3/T]) is composed of a series successive control volumes.

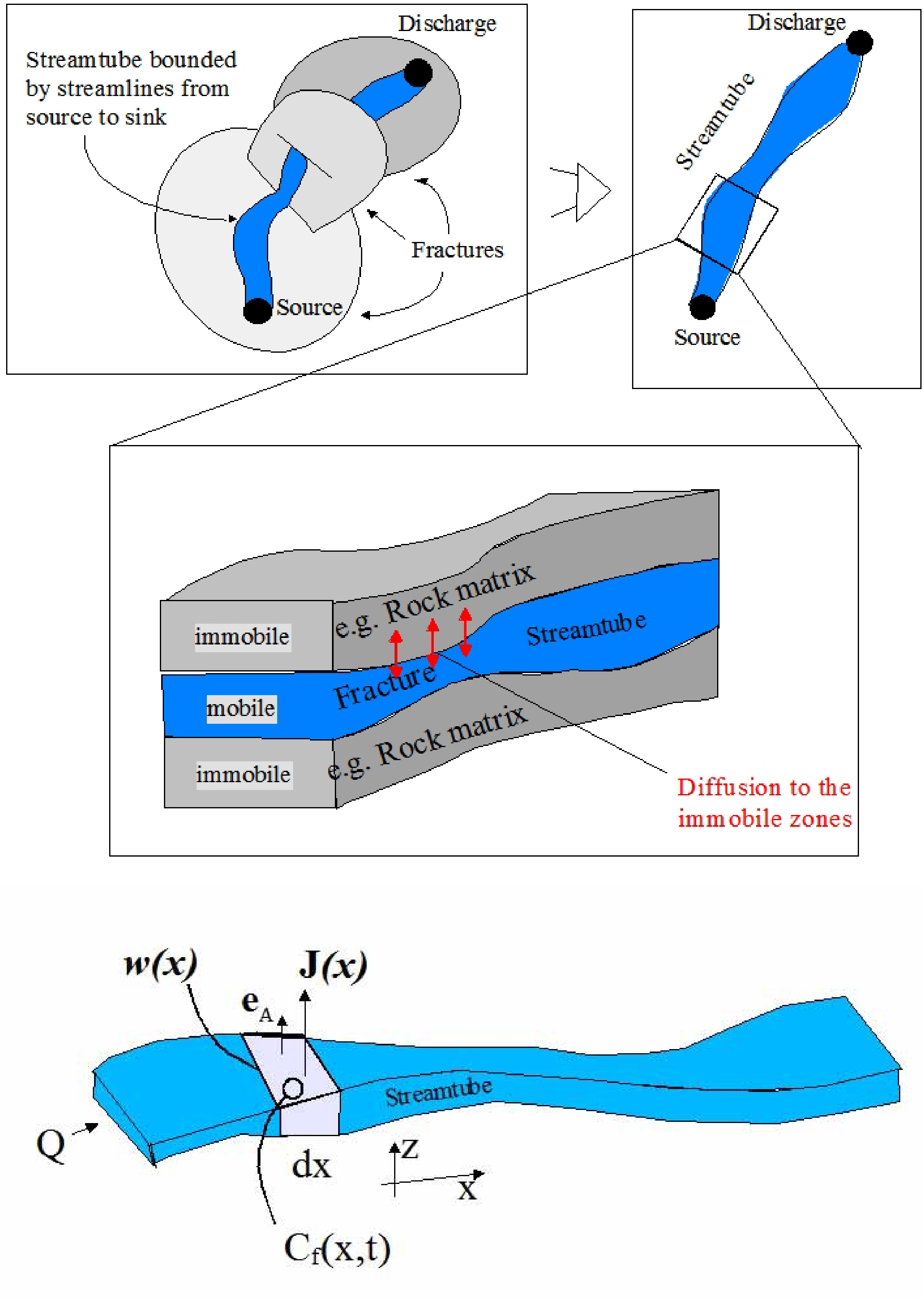


Figure 1. *Streamtube and a control volume used to assess the mass balance equation for the solute transport. The control volume is indicated by the gray colour in the graph at the bottom. Symbols indicated in the figure refer to the equations in the text and are explained in that context.*

The mass balance equation of the solute transport can be deduced to be

$$R_a \frac{\partial m(x,t)}{\partial t} = Q\left[C_f(x,t) - C_f(x+dx,t)\right] - \vec{J}(x,t;z=0)\cdot \vec{e}_A W(x)\,dx\,, \tag{1}$$

where m [M] is the solute mass in the control volume, C_f [M/L^3] is the solute concentration in the control volume and the streamtube is characterised by the width $W(x)$ [L], volume aperture $2b(x)$ [L] and flow rate Q [L^3/T] and $\vec{e}_A$ [-] is the outer normal of the control volume at the diffusion interface. Equilibrium sorption types of interactions with the surfaces are represented by the retardation factor R_a [-]. All properties depend on the location (except Q that defines the streamtube), i.e. there is heterogeneity along the flow path and in the immobile zone. The diffusional mass transfer between the immobile zone and the streamtube is described by the flux $\vec{J}$ [M/T/L^2] presented in equation (2).

$$\vec{J}(x,t,z) = -D_e(x,z)\frac{\partial C_m(x,t,z)}{\partial z}\vec{e}_z \quad , \tag{2}$$

where D_e [L^2/T] is the effective diffusion coefficient of the immobile zone and C_m [M/L^3] is the solute concentration in the pore water of the immobile zone.

In the immobile zone the solute mass transfer is governed by the diffusion as indicated by the equation (3)

$$R_p \frac{\partial C_m(x,t,z)}{\partial t} = D_p(x,z)\frac{\partial^2 C_m(x,t,z)}{\partial z^2} \quad , \tag{3}$$

where R_p [-] is the retardation coefficient in the immobile zone and D_p [L^2/T] is the pore diffusivity in the immobile zone. We require continuity of the solute concentration over the control volume and immobile zones. This means that

$$C_m(x,t,z=0) = C_f(x,t) \quad . \tag{4}$$

Note, that Equation (4) is simplified by stating C_m=C_f at z=0 instead of z=$b(x)$. These are equivalent formulations because it is assumed that well mixed conditions prevail in the fracture, i.e. C_f does not depend on z. In this case z measures the distance from the fracture wall, not from the centreline of the fracture.

It is convenient to describe the condition (4) by representing the solute concentration in the matrix as it is shown in the equation (5) and (6)

$$C_m(x,t,z) = g(x,t,z)\,C_f(x,t) \tag{5}$$

$$g(x,t,z=0) = 1 \quad . \tag{6}$$

Diffusional mass transfer in the immobile zone can now be represented using flux

$$\vec{j}(x,t,z) = -D_e(x,z)\frac{\partial g(x,t,z)}{\partial z}\vec{e}_z \ . \tag{7}$$

Diffusion flux in equation (1) can be written as

$$\vec{J}(x,t,z) = C_f(x,t)\,\vec{j}(x,t,z) \tag{8}$$

and the mass balance equation (1) is modified to

$$R_a \frac{\partial C_f(x,t)}{\partial t} = -\frac{Q}{W(x)\,2b(x)}\frac{\partial C_f(x,t)}{\partial x} - \frac{C_f(x,t)}{2b(x)}\,j(x,t,z=0) \quad . \tag{9}$$

In order to examine some of the main properties of this transport equation it is not necessary to specify the structure and boundary conditions of the immobile zone, i.e. it is not necessary to solve equation (3), as it will become evident through the examination of the equation (9).

First, we take a Laplace transform of the equation (9) in respect of time

$$R_a s\ \widetilde{C}_f(x,s) = -\frac{Q}{W(x)\,2b(x)}\frac{\partial \widetilde{C}_f(x,s)}{\partial x} - \frac{\widetilde{C}_f(x,s)}{2b(x)}\,\widetilde{j}(x,s,z=0)\ , \tag{10}$$

where tilde denotes Laplace transformation and s of the variable of the Laplace transformed domain. Equation (10) is solved for the initial condition of a sudden release of mass M_0 at the inlet of the streamtube, i.e.

$$\begin{aligned} &C_f(x=0,t) = \frac{M_0}{Q}\delta(t) \rightarrow \widetilde{C}_f(x=0,s) = \frac{M_0}{Q} \\ &C_m(x,t=0,z) = C_f(x,t=0) = 0 \end{aligned} \tag{11}$$

The Laplace transform of the solute mass flux at the outlet of the streamtube (x=L) is

$$\begin{aligned} \frac{\widetilde{m}(L,s)}{M_0} &= \frac{Q}{M_0}\widetilde{C}_f(x,s) = \mathrm{Exp}\left[-s\int_0^L R_a \frac{W(x)2b(x)}{Q}dx - \int_0^L \frac{W(x)\widetilde{j}(x,s,z=0)}{Q}dx\right] \\ &= \mathrm{Exp}\left[-s\,R_a\frac{V}{Q} - \int_0^L \frac{W(x)\widetilde{j}(x,s,z=0)}{Q}dx\right] \end{aligned}\ , \tag{12}$$

where the volume of the flow channel is denoted by $V = \int_0^L W(x)2b(x)dx$. It is also easy to see from equation (12) that if the equilibrium sorption R_a depends on the location along the flow path then the advection-equilibrium sorption term is $\int R_a(x)W(x)2b(x)/Q\,dx$ instead of the $R_a V/Q$.

It is noted from the equation (12) that besides the advective delay, *V*/*Q*, the solute discharge depends on the entity

$$u = \int_0^L \frac{W(x)\tilde{j}(x,s,z=0)}{Q}dx \quad . \tag{13}$$

The *u* in equation (13) depends on the flow field and diffusion to the immobile zones. Similar derivations have been presented, for example, for a number of different infinite immobile zones by Neretnieks (e.g. 2002) and for heterogeneous flow paths by Cvetkovic et al. (1999). The present formulation shows that the coupling to the flow field is applicable even for a general case of non-prescribed diffusion flux $\tilde{j}(x,s)$. The measures of the flow field that control the coupling to the matrix diffusion do not depend on the structure of the immobile zones.

The flow dependent part $\int W(x)/Q\,dx$ is also called as the hydrodynamic control of retention and it is denoted by many different notations: e.g. β, WL/Q (in TILA-99), FWS/Q (flow-wetted-surface divided by the flow rate) or F-Factor. Generally accepted equivalences between the notations are $\beta = F = FWS/Q = 2WL/Q = 2\int W(x)/Q\,dx$.

3.2 Heterogeneity along the flow path

Equation (13) indicates that both flow field and diffusional coupling to the immobile zone are important for the assessment of the retention. Transport properties along a heterogeneous flow path can be examined by assuming that the local properties W(x)/Q and $\tilde{j}(x,s,z=0)$ are random variables along the path. We may represent these random variables by mean values and perturbations around the mean values

$$\begin{aligned} &\frac{\mathbf{W}}{\mathbf{Q}} = \left\langle \frac{W}{Q} \right\rangle + \left(\frac{W}{Q}\right)', \quad \left\langle \left(\frac{W}{Q}\right)' \right\rangle = 0 \\ &\tilde{\mathbf{j}}(\mathbf{s},\mathbf{z}=\mathbf{0}) = \left\langle \tilde{j}(s,z=0) \right\rangle + \tilde{j}(s,z=0)', \quad \left\langle \tilde{j}(s,z=0)' \right\rangle = 0 \end{aligned} \quad , \tag{14}$$

where $\langle \; \rangle$ indicates spatial average along the flow path and the apostrophe denotes perturbation . Substituting expressions in equation (14) to the equation (13) gives

$$u = \int_0^L \frac{W(x)\tilde{j}(x,s,z=0)}{Q}dx = \left\langle \frac{W}{Q} \right\rangle \left\langle \tilde{j} \right\rangle L + \left\langle \frac{W}{Q}\tilde{j} \right\rangle L \quad . \tag{15}$$

This means that, if there is no correlation between the local flow property W/Q and the diffusional mass transfer to the immobile zone, then average values can be used to calculate *u*, i.e.

$$u = \int_0^L \frac{W(x)\tilde{j}(x,s,z=0)}{Q} dx = \left\langle \frac{W}{Q} \right\rangle \left\langle \tilde{j}(s,z=0) \right\rangle L, \quad \text{if} \left\langle \frac{W}{Q} \tilde{j} \right\rangle = 0 \quad . \tag{16}$$

In the case of equation (16) it is possible to estimate the flow part, $\langle W/Q \rangle L$, separately and apply it later in the transport program, which incorporates the flow part with the average diffusional mass transfer, $\langle \tilde{j} \rangle$. This assumption has been applied in many performance assessments, for example in the Posiva's TILA-99 analysis and in the SKB performance assessment SR97.

In many cases there may be correlations between the local flow and diffusion properties depending e.g. on the fracture or structure types that are visited along the flow path or on the groundwater chemistry in the immobile pores. For example, it is usual that the rock matrix is more altered in fracture zones than around the background fractures that affects the local solute diffusion to the immobile zones. It also appears that the flow rates are higher in the fracture zones than in the background fractures, i.e. there can be a correlation between the local flow and diffusion properties if the flow path goes through both background fractures and fracture zones.

The possible correlations along the flow paths can be taken into account and still apply the simple averaged values as in the equation (16). This can be worked out by classifying flow path to different flow and diffusion environments. This is illustrated later in *Figure 7*. Let us assume that there are *n* types of fractures and that in each fracture type diffusion properties are non-correlated with the flow property. The fracture classes can be, for example, background fractures and fracture zones. Equation (15) can now be written as

$$u = \sum_{j=1}^{n} \int_{L_j} \frac{W(x)}{Q} \tilde{j}_j(x,s,z=0) dx = \sum_{j=1}^{n} \left\langle \frac{W}{Q} \right\rangle_j L_j \left\langle \tilde{j}(x,s,z=0) \right\rangle_j , \qquad \sum_{j=1}^{n} L_j = L . \tag{17}$$

The flow path is here divided into piecewise uncorrelated parts. The benefit of this approach is that the flow properties $\langle W/Q \rangle_j L_j$ can be assessed independently of the assessment of the diffusion properties. The coupling of the local diffusion and flow properties is replaced by appropriate bookkeeping that can be used in the radionuclide transport calculations to reproduce the flow path.

3.3 Several parallel immobile zones along the flow path

In many cases the streamtube (flow path) can be in contact with several different types of immobile zones because of the heterogeneity in the immobile zone properties. A typical example could be a streamtube alongside with a stagnant pool or fault gouge. In this case solute particles can access the immobile zones directly from the streamtube and through the stagnant areas in the fracture plane, i.e. stagnant pools or fault gouge. The additional alternative access to the immobile zones may provide considerable add to the overall retention. Conceptually this can be described by supplementing *Figure 1* as it is shown in the Figure 2.

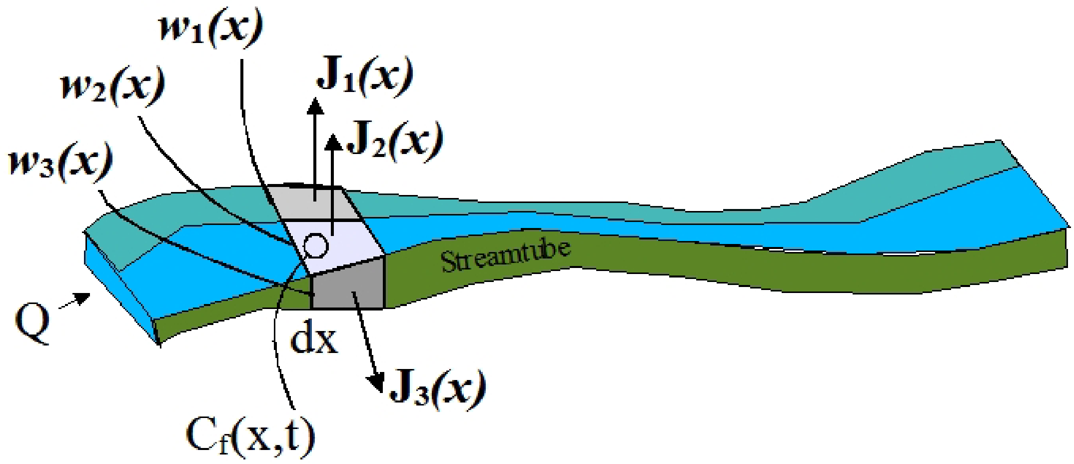


Figure 2. *Streamtube and a control volume used to assess the mass balance equation for the solute transport in case of several parallel immobile pore spaces.*

It is now quite straightforward to change equation (1) to take into account m parallel diffusion processes (although, in practice usually $m \leq 2$)

$$R_a \frac{\partial m(x,t)}{\partial t} = Q\big(C_f(x,t) - C_f(x+dx,t)\big) - \sum_{i=1}^{m} \vec{J}_i(x,t;z=0)\cdot \vec{e}_A\, w_i(x)\, dx \ . \tag{18}$$

The measure of width across the diffusion interface is now denoted by lowercase $w_i(x)$ in order to separate it from the width $W(x)$ that defines the 2D Darcy velocity along the streamtube in the fracture planes. Naturally, for the diffusion directly from the streamtube to the rock matrix $w_i(x)=W(x)$.

The minor addition in equation (18) can be carried out to the solution in equation (12) that in this case reads

$$\frac{\widetilde{m}(L,s)}{M_0} = \mathrm{Exp}\left[-R_a\, s \frac{V}{Q} - \sum_{i=1}^{m} \int_0^L \frac{w_i(x)\widetilde{j}_i(x,s,z=0)}{Q} dx \right] \quad . \tag{19}$$

Applying this to the estimated flow property (equation (17)) yields

$$u = \sum_{j=1}^{n}\sum_{i=1}^{m}\int_{L_j}\frac{w_i(x)}{Q}\tilde{j}_{ij}(x,s,z=0)dx$$

$$= \sum_{j=1}^{n}L_j\sum_{i=1}^{m}\left\langle\frac{w}{Q}\right\rangle_{ij}\left\langle\tilde{j}(x,s,z=0)\right\rangle_{ij}, \qquad \sum_{j=1}^{n}L_j = L \quad , \tag{20}$$

In the typical example of the direct diffusion to the rock matrix and parallel diffusion through the stagnant pools is represented by m=2 and the couplings are $\langle w/Q\rangle_{1j} = \langle W/Q\rangle_j$ and $\langle w/Q\rangle_{2j} = \langle 2b/Q\rangle_j$.

3.4 Application of the numerical flow solution

In practice, numerical flow solutions are rarely suitable for direct application of equations (13), (17) or (20). Equations (12) and (13) are derived for a well mixed streamtube that carries a fixed flow rate. However, in the numerical calculations it is not usually possible to discretize the model by following the streamtubes. Discretization of the numerical models may overlap with several streamtubes or if the discretization is detailed enough they provide local samples of the streamtubes.

In the numerical flow model there is no physical process that is able to average the flow field, contrary to the solute transport in which the molecular diffusion averages the flow field. In this respect, over the element size averaged flow provided by the numerical flow solution fits well for the estimation of the hydrodynamic control of retention, i.e. the flow dependent part of the equation (17) ($\langle W/Q\rangle_j L_j$). This requires that the resolution of the numerical solution is suitable compared with the corresponding transport problem.

In the numerical flow model the streamtube is followed by e.g. particle paths along the fractures (cf. illustration in *Figure 6* and a simulation example in *Figure 10*). In this case, equation (17) can be rewritten in the form

$$u = \sum_{j=1}^{n}\left\langle\frac{W}{Q}\right\rangle_j^e L_j\left\langle\tilde{j}(x,s,z=0)\right\rangle_j, \qquad \sum_{j=1}^{n}L_j = L \quad , \tag{21}$$

where the superscript e implies that the average is taken over the element and not along the streamtube. In addition, the summing in equation (17) was over the different fracture types (i.e. different immobile zone types). In equation (21) the summing goes over the elements visited along the particle path. Naturally, this summation can also be used for the bookkeeping of the fracture and immobile zone types along the flow path. It seems clear that if the discretization is too coarse it will cause averaging over several streamtubes that will distort the results. Especially, averaging over different fractures need to avoided because the flow properties in different fractures can be totally different.

Replacing the averages over the streamtube by averages over the element lends itself well to the more general case of several parallel immobile zones. As in the equation (21), summation and averaging is made over the elements visited along the flow path

$$u = \sum_{j=1}^{n} L_j \sum_{i=1}^{m} \left\langle \frac{w}{Q} \right\rangle_{ij}^{e} \left\langle \tilde{j}(x,s,z=0) \right\rangle_{ij}, \qquad \sum_{j=1}^{n} L_j = L. \tag{22}$$

There are also problems related to the equation (22). The coupling between the flow field and diffusion to the immobile zones is given by the factors $\langle w/Q \rangle_{ij}^{e}$. The 2D flow solution of the fracture flow gives the Darcy velocity on the fracture plane $\langle Q/W \rangle_{ij}^{e} = 1/\langle W/Q \rangle_{ij}^{e}$. This means that if the immobile zones are perpendicular to the fracture plane, then the flow solution can be used to approximate the coupling factor. If the element size is small enough then this approach is also able to take into account the channelling of the flow in heterogeneous fractures.

3.5 Required resolution of the flow field

It is assumed that the solute concentration in the streamtube is well mixed. Especially, this is important in the direction of the diffusion to the immobile zone, because in that case the concentration gradient affects both advective flux of the solute along the fracture and diffusion to the immobile zones. In this respect, diffusion from the streamtube directly to the rock matrix is not a problem because the fracture apertures are so small that, in practice, the solute concentration is always well mixed in the direction of the fracture aperture.

Diffusion in the fracture plane determines the averaging over the flow field. Neretnieks (2002) has considered diffusional mixing in the flow field for the case where two flow paths are in contact with each other. It appears that diffusional mixing is not very pronounced. Well mixed conditions can be estimated using equation $l = 2.2\sqrt{Dt}$, where l represent channel width over which the streamlines have lost their identity, D is the molecular diffusivity in free water and t is time. This gives channel width of about 20 cm if the mixing takes place for a one year. Advective travel time through a 500 m long parallel plate fracture ($T=10^{-7}$ m^2/s) for a 0.1 % hydraulic gradient is about 8 years. Based on this data it can be concluded that at most the mixing takes place over some tens of centimetres.

The rather weak mixing also means that there are good reasons to assume that the streamtubes are independent and that they can be modelled as one dimensional channels (cf. also Neretnieks, 2002).

4 CONCEPTUALISATION OF THE FLOW

This section discusses different options for conceptualisation of the flow in bedrock. Section 3 shows that the flow dependent retention properties reflect the fractured character of the rock and they also depend on the local flow rate along the flow path. Calculation of the retention properties should be based on the assessment of the flow field (transport channels) at an appropriate level of details.

At least three different flow environments can be identified: channelling that cause variable flow in the individual fracture planes, transmissivity differences between the fractures leading to preferential flow paths through the fracture network and extensive fracture zones providing highly transmissive connection over long distances. This suggests that flow needs to be described at the level of individual fractures, in some cases possibly even in a smaller scale determined by the channelling of the flow. Heterogeneity is important in all scales indicating that the model size should be comparable to expected transport distances.

4.1 Continuum models

Continuum models (EPM, Equivalent Porous Medium) apply average properties of the rock to model the groundwater flow. In practice, this means that the varying flow field over large numbers of interconnected fractures is replaced by an effective conductivity.

Benefits of the continuum approach are that they are usually computationally feasible so that they can cover large volumes of rock and assessment of the transport paths can be implemented easily. Transport paths are usually conceptualised as imaginary one-dimensional streamtubes. Properties of both flowing fractures and immobile pore space are averaged over the block size of the model and these averaged properties are applied along the streamtubes.

The continuum models may also explicitly include deterministic large scale hydraulic zones. In that case the averaging is only applied for the stochastic and small scale heterogeneity. Continuum model may also include a stochastic component. In the stochastic continuum models the block conductivities are drawn from statistical distributions. This increases heterogeneity of the model and facilitates simulation of the natural variability of the fractured rock.

Continuum models are powerful for the assessment of the overall flow conditions. In the assessment of the transport and retention properties the main problems are connected to the averaging of the transport properties over large volumes. Up-scaling of the retention properties takes place already at the averaging scale of the model, i.e. in the scale of the elementary blocks of the model. The underlying heterogeneity of the fractured rock implies that the averaged estimate of the retention property may lead to overestimation of the solute retention.

4.2 Fracture network models

Fracture network modelling (DFN, Discrete Fracture Network) tries to mimic the structure of the fractured rock by explicitly including fractures to the model. The flow model is constructed so that the groundwater flow takes place through the network of interconnected fractures. Usually, the rock between fractures is not even included to the flow model.

Fracture network models describe the groundwater flow and transport properties by incorporating huge amount of details to a stochastic model. It is not possible to deterministically characterise all fractures to the level of details that is required in the transport calculations. The fracturing is represented using probability distributions for fracture frequency, sizes, orientations and transmissivities. However, the stochastic nature of the fracture network models does not preclude addition of the deterministic features to the model. Known large-scale hydraulic features are usually represented deterministically in the model.

Averaging of the flow and transport properties in the fracture network model takes place in a different scale than in the continuum models. In the fracture network model the hydraulic properties are usually averaged in the scale of the individual fractures; not over blocks of fractures as it is the case in the continuum models.

Main problems with the fracture network models are connected to the computational feasibility. The number of fractures is usually directly proportional to the volume of the modelling domain. Commonly, the number of fractures limits the size of the model due to the computational constrains.

4.3 Comparison of the approaches

Transport and retention properties are dependent on the flow properties along individual flow paths. This differs from the characteristics of the overall flow conditions that can be described by the average flow rates in the block scale. In practice, this favours application of the DFN modelling for the assessment of the transport and retention properties.

Application of the continuum approach on the transport and retention calculations requires appropriate down-scaling methods for the estimation of the detailed scale flow measures. Many different approaches have been developed for that purpose. For example, Öhman et al (2005) use the fracture network model to obtain the flow and transport statistics at an appropriate support scale. The support scale is selected so that flow can be represented by means of a continuum. Stochastic continuum flow simulation is applied in combination with particle tracking to model large-scale transport. Detailed fracture scale properties are transferred to the regional scale using the block scale description. Painter and Cvetkovic (2005) employs site specific fracture network modelling as a tool to assess the statistical properties of the transport pathways for a subdomain of the site scale domain. The simulated statistics is then applied for the assessment of the transport over longer pathways.

Common to most of the approaches is that in the detailed scale they need to be based on the fracture network representation of the fracturing. An important assumption is that the fracture network model used in the simulations is also representative for the fracture network in the larger scale, or in other words, that the fracturing is statistical homogeneous over a larger volume of the rock than is applied in the down-scaling DFN simulations. This assumption is jeopardised by the fact that there is heterogeneity in all scales of the rock. In practice, this means that statistics of the small scale DFN model is not able to fully extrapolate the influence of the larger zones in the larger scale. However, both Öhman et al (2005) and Painter and Cvetkovic (2005) present methods that reduces the possible inconsistency between the down-scaling approximation of the transport properties and application of them in the larger scale by e.g. favouring persistency in the properties of the flow paths.

The heterogeneity in all scales has an important implication to the transport and retention properties. Therefore, the present transport concept is based on application of the site scale DFN model. Computational feasibility is ensured by focusing the detailed scale fracturing only to the regions of the model that have active flow paths.

5 THE CONCEPT FOR TRANSPORT CALCULATIONS

This section introduces the concept applied for the radionuclide transport calculations. The main emphasis is on the simulation of the transport and retention properties using different flow models. Alternative options for the coupling between the flow modelling and radionuclide transport calculations are also outlined. Flow modelling techniques are not a subject of this report and they are not discussed any further than is needed for understanding of the assessment of the transport and retention properties.

5.1 Approach

The basic structure of the fractured rock leads to very uneven distribution of the flow between different hydraulic features (see Section 2). Preferential flow paths and channelled transport can be observed in all scales. This needs be taken into account in the simulations of the transport and retention properties. This can be done by explicitly modelling fractures in all scales along the flow paths and applying models using appropriate spatial resolution. In practice, this leads to a site scale DFN model that is composed of hydraulic structures in very different scales. The model includes at least regional scale, site scale and fracture scale hydraulic features (see Figure 3).

Another important requirement to the transport and retention simulations is that they need to support understanding of the performance of the geosphere as a migration barrier. This calls for transparent modelling that sheds light on the different components of the overall retention along the flow paths. In the transport and retention simulations this is supported by application of alternative models to address different processes.

Transport and retention analysis are divided to two different approaches which both are based on the DFN modelling:

- Steady state simulations. This is the main part of the simulations and the approach that is also outlined in the safety case plan. Radionuclide transport calculations are separated from the evaluation of the flow related transport and retention properties. Evolving flow conditions are modelled by “snapshots” in time. This methodology has many advantages: assessment of the flow conditions is not confined to any particular approach of the radionuclide transport calculations, it is easy to perform simplified analysis to bound the uncertainty analysis, conservative assumptions can be applied in a controlled way at the phase of the radionuclide transport calculations and the approach is transparent because the flow dependent component is modelled separately.

- Transient simulations. Transient modelling of the radionuclide transport in the evolving flow field requires integration of the flow and radionuclide transport models. Posiva is presently taking part to the model development that aims to transient transport modelling tool (computer program Marfa, see Appendix A). Transient simulations are applied in support of the steady state simulations. Note, that steady state simulations can also take into account transient features of the flow field e.g. changes in the flow rates along the flow paths.

Steady state and transient simulations are discussed further in Sections 5.3 and 5.4.

Transport and retention simulations are focused on the flow field, but they should also provide information on the retention properties of the fractures along the flow paths. In the transport concept this is resolved so that a few generalised retention models are developed based on the geological information collected from the fractures. Fractures of the site scale DFN model are classified according to the retention model. Retention model types along the flow paths are recorded during the DFN flow analysis and the collected information is delivered to the radionuclide transport simulations. Generalised retention models are discussed more in detail in Section 5.2.

Table 1 and *Figure 4* summarizes modelling approaches and tools that can be applied to study the different components of the geosphere retention.

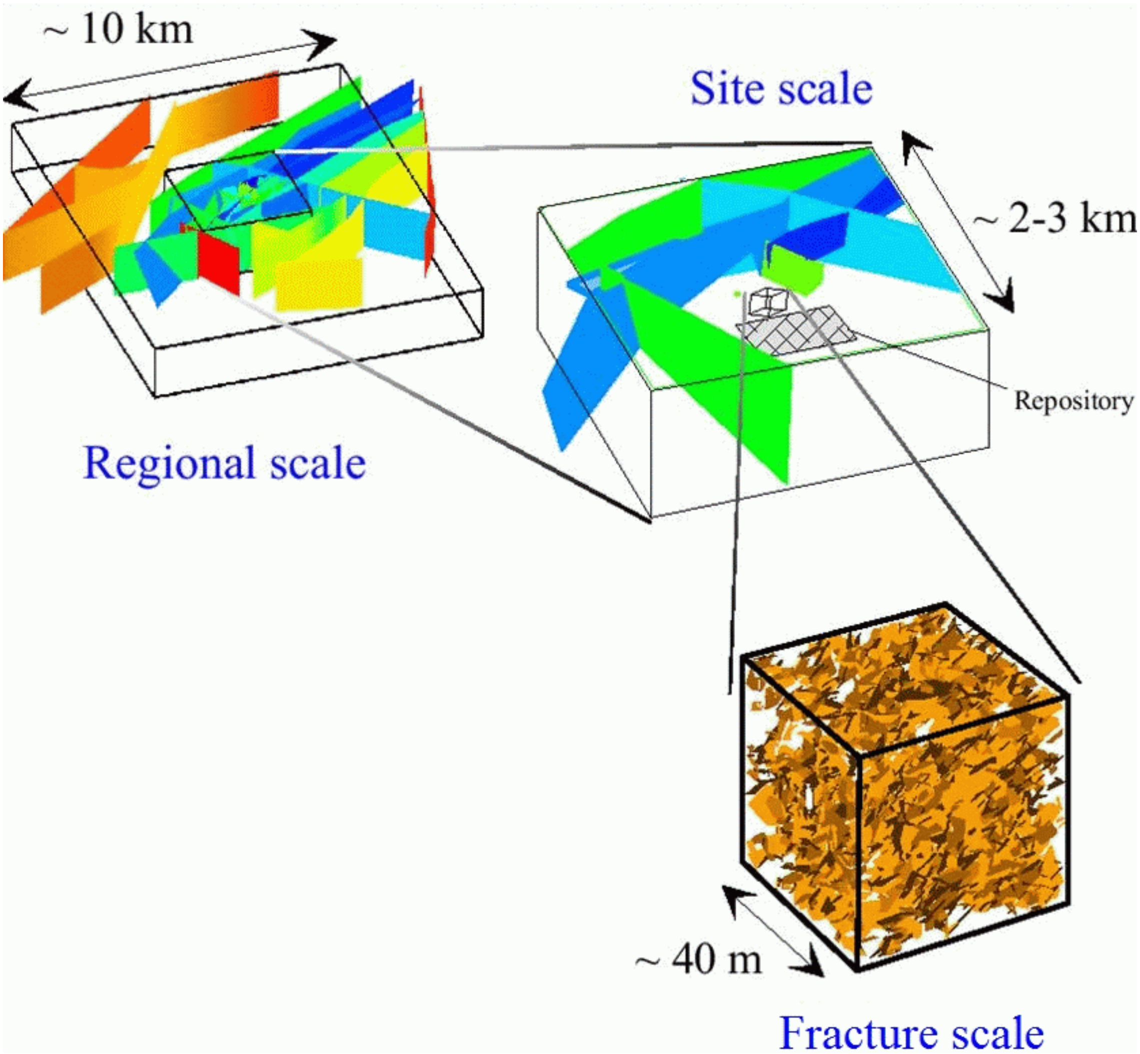


Figure 3. *Fractured rock is heterogeneous in all scales. Hydrological features can be divided to regional scale, site scale and fracture scale features. All scales can be important in the transport and retention analysis.*

Table 1. *Models applied for the simulations of the transport and retention properties and for the radionuclide transport calculations. Computer programs are introduced in the Appendix A.*

Process or feature	**Analysis of the transport and retention properties**	**Radionuclide transport calculation**	**Required data**
Snapshot in time	ConnectFlow (DFN) FEFTRA+ VINTAGE (DFN) Simplified analytical (part of the uncertainty analysis)	Marfa FTRANS Simplified analytical (part of the uncertainty analysis)	Hydro-DFN data Retention models Sorption data Boundary conditions FEFTRA (EPM) analysis of the evolving flow conditions
Transient flow paths	ConnectFlow (DFN)	Marfa	Hydro-DFN data Retention models Sorption data Boundary conditions Site evolution

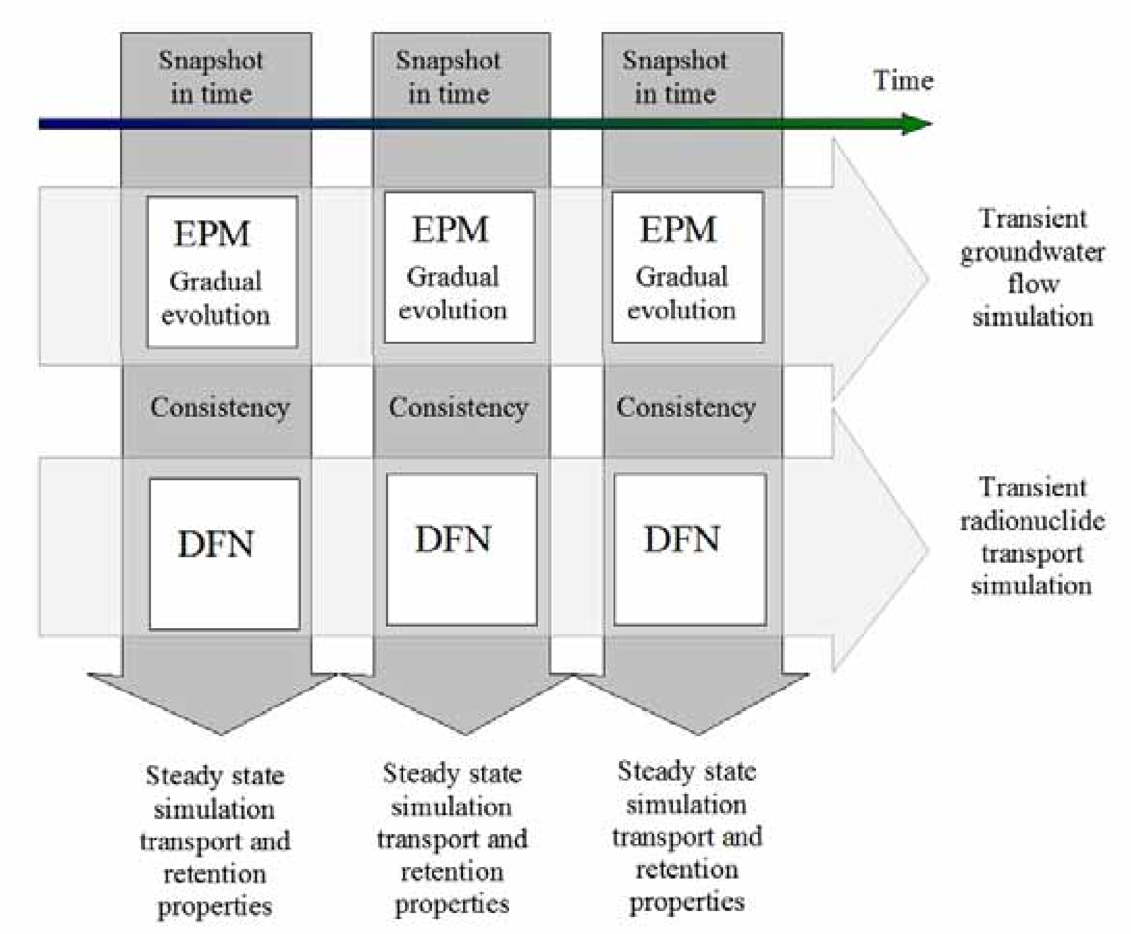


Figure 4. *Transport and retention properties are simulated using both steady state and transient simulations.*

Figure 4 illustrates how the time evolution is taken into account in the flow and transport modelling. EPM flow modelling is based on the transient groundwater flow simulations. However, flow paths are analysed for snapshots in time. Assessment of the transport and retention properties is based on the DFN modelling that is not simulating the fully transient evolution of the site, because all processes (e.g. density dependent flow) are not available in the DFN modelling as they are in the EPM modelling. DFN modelling follows the same pattern of snapshots in time that are used in the flow path analyses of the EPM modelling and these DFN snapshots are used for assessment of the transport and retention properties. This also offers an opportunity to check consistency between EPM and DFN models for the few snapshots in time. Finally, the time series DFN models can be used for a transient type of analysis that is composed of a few steady state flow fields simulated for evolving boundary conditions.

5.2 Generalised rock matrix retention models

Generalised retention models are based on the conceptualisation and parameterisation of the immobile zones next to the different types of fractures or hydraulic features. Definition of the retention models should be based on the geological data and understanding of the site specific features of the fracturing. In practice, the retention model describes structure and capacity of the geological materials, like fault gouge, rock matrix alterations and unaltered rock matrix that are next to the fracture or the flow channel in the fracture. The rock matrix and geological materials are specified and quantified in respect of the main retention parameters, i.e. sorption, porosity and diffusivity.

The number of different retention models depends on the site specific features, but the number of different retention models is foreseen to be low because of the large geological variability. Due to the natural variability between fractures it is likely that the retention models will capture only major differences between the fractures.

The retention model does not affect on the groundwater flow, but it is essential for the radionuclide transport calculations. Application of the retention models can reduce the need for conservative assumptions in the transport calculations and they can support realistic assessment of the performance of the geosphere as a migration barrier. Retention models can also serve a basis for the further simplification and parameterisation of the immobile zone properties, for example, in the bounding calculations of the uncertainty analysis.

The DFN flow analysis treats the different retention models as any additional property of the fractures. Flow path analysis keeps book on the retention model types by recording it when a fracture is visited by the flow path. The recorded information is given to the radionuclide transport calculations.

An example of the generalised retention models are the microstructural models of the fractures developed for the Äspö Hard Rock Laboratory (Dershowitz et al. 2003). Based on the geological characterisation fractures are divided to two generalized fracture types: Type 1 (faults) and Type 2 (joints). The microstructural model comprises description and full parameterisation of the immobile zones for the two fracture types. *Figure 5* exemplifies the definition of the immobile zones for the two fracture types.

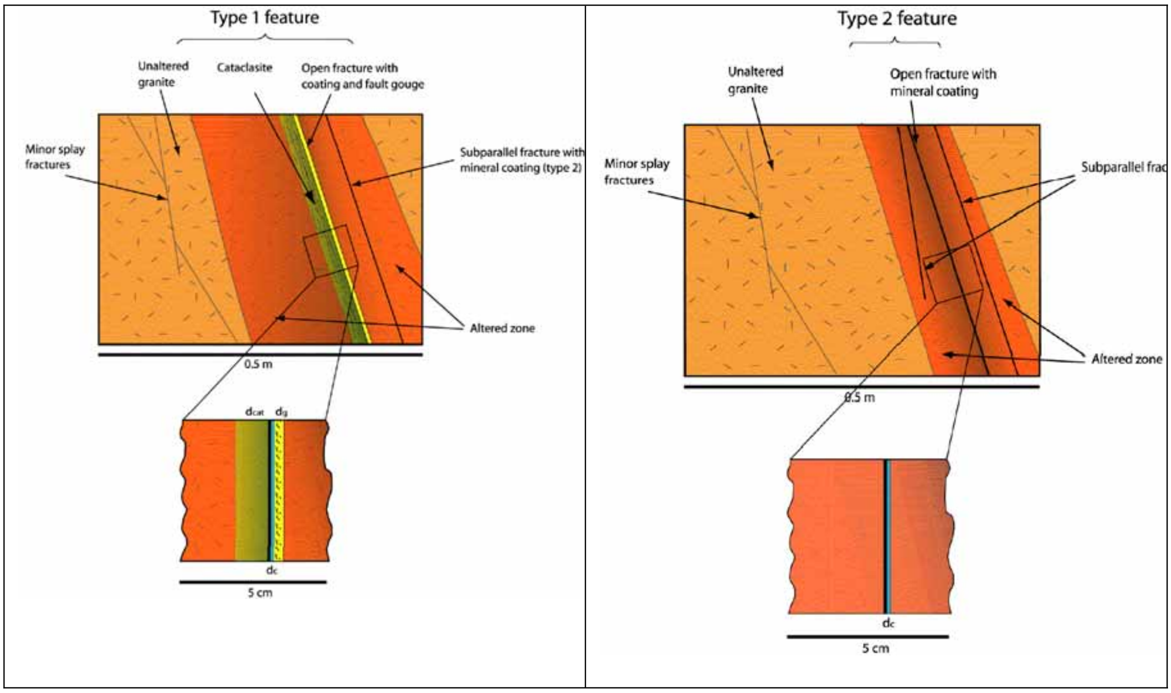


Figure 5. *An example of the generalised retention models for two different fracture types (from Äspö Hard Rock Laboratory, Dershowitz et al., 2003).*

5.3 Steady state simulations

The major part of the transport and retention simulations are carried out for the steady state simulations of the flow paths. In this approach the radionuclide transport calculations are executed in the separate simulations based on the one-dimensional transport channels. Transport channels are represented by the flow paths that are determined and analysed by a steady state DFN flow model.

This kind of approach has been applied for the radionuclide transport calculations in many previous safety assessments. Enhancements of the present approach compared to the previous analyses are:

- Site evolution is taken into account. The flow conditions are analysed and a suitable set of distinct flow conditions are analysed by the steady state model as "snapshots" in time.
- Heterogeneity of the fractured rock is taken into account by explicitly including small scale fracturing into the model where it is appropriate.
- Heterogeneity of the rock mass and geological materials is taken into account by taking advantage of the generalised retention models.
- Varying sorption properties, in space or in time, can be taken into account. This requires interplay between the radionuclide transport calculations and the flow simulations.

- Time dependent flow rates can be taken into account. Actually, this is a property of the radionuclide transport calculations, but the flow analyses can be designed to support this option. Varying flow rates do not implicate fully transient modelling, because the geometries and composition of the transport paths remain unchanged during the modelling period.

5.3.1 Flow model

Assessment of the retention properties differs from the modelling of the overall flow conditions. Overall flow conditions can be modelled by averaging the background fracturing over three dimensional blocks of rock and applying continuum models (EPM and/or SC). Averaging makes it possible to model large volumes of rock that in turn enables application of the reliable boundary conditions. Assessment of the retention properties need to be based on the flow rates along individual flow paths, instead of the total flow rates. In practice, this means that DFN modelling need to be applied to analyse flow properties along the flow paths.

Flow conditions around the repository will evolve in a short time perspective due to disturbances caused by the repository itself (saturation of the tunnel backfill and buffers, chemical disturbances, recovery of the water table) and in a longer time perspective due to, for example, post glacial land up-lift and possible climate changes. Evolution of the flow field is influenced by a number of processes that are not straightforward to couple with the detailed DFN flow model. Detailed description of the fractures requires large amount of computing resources. Therefore, for example, the rock mass between the fractures is usually omitted from the DFN flow model. This means that it is almost impossible to use DFN flow model to simulate some of the processes, like effects of the heat produced in the disposal canisters.

It seems evident that the gradual evolution of the groundwater flow with full coupling to the processes that may affect the groundwater flow need to be examined mainly by the EPM models. The EPM flow modelling provides general characteristics of the flow conditions for different periods of the time. This information can be used to make well justified choices about the few "snapshots" in time that are simulated using the DFN flow model and analysed by the transport modelling. The role of the DFN modelling can be seen, not merely as an alternative flow modelling approach, but a tool that is used to determine the distribution of the overall flow to the individual fractures and flow paths.

Hydraulic properties of the detailed scale cannot be fully identical in the DFN and EPM models. The hydraulic behaviour of the background fracturing is more heterogeneous and usually also more anisotropic in the DFN model than in the more averaged EPM model. Therefore, it is important to cross-check the DFN modelling results with the corresponding EPM modelling results. This ensures that the state of the flow conditions is reproduced consistently enough by the DFN and EPM models. The key properties of the flow conditions that need to be compared are the site scale flow paths and block size flow rates. Possible disparity between the models needs to be explained and reduced by appropriate changes in the boundary conditions and/or effective hydraulic properties. At least, consequences of the disparity in the flow conditions to the transport properties and performance of the geosphere need to be assessed. In practice, this means that the interplay between the gradually evolving EPM model and the "snapshot" type DFN model is an iterative process.

The steady state simulations can also be applied to analyse the operational phase of the repository and the inflow paths to the repository tunnels. This extends the applicability of this approach to link between the hydraulic and geochemical modelling of the disturbances caused by the repository.

Roles of the EPM and DFN modelling are summarised in *Table 2*.

Table 2. *Roles of the EPM and DFN flow modelling in the assessments of the flow related transport properties.*

Process	**EPM**	**DFN**
Density dependent flow	Full coupling	Density driven flow (distribution of the salt from the EPM modelling). No transport of salt
Land up lift	Yes	Steady state (snapshot in time)
Heat production in deposition canisters	Yes	No
Major fracture zones (deterministic)	Yes	Yes
Large fracture zones	Averaged to 3D background conductivity	Stochastic
Background fractures	Averaged to 3D background conductivity	Stochastic
Engineered structures	Yes	Yes
Heterogeneity within fractures / zones	No	Optional

5.3.2 Transport channels

Transport channels can be treated as a bundle of one dimensional individual conduit if there is no mixing between the channels (Bear et al., 1993). Assumption of the weak mixing between the channels has been commonly applied in the performance assessment modelling and transport is simulated for independent channels. Examination of the flow conditions in the fractured rock supports this conclusion (cf. Section 3.5).

The present transport concept takes advantage of the one dimensional nature of the solute transport through the fractured rock. In practice, this means that the transport channels are identified by particle tracking using the simulated DFN flow field. Starting locations and the number of release paths should give a statistically adequate view of the potential flow paths. Precise number of the flow paths and starting locations are agreed with the performance assessment.

The role of the groundwater flow simulation is to characterise the flow paths that are used as transport channels in the radionuclide transport calculations. Basis of the transport calculations is the site scale DFN flow model. Each transport channel is composed of segments that are the finite elements of the DFN flow model visited by the flow path. Each segment is characterised by the retention model and the corresponding flow property as indicated in Figure 7. An overview of the assessment of the transport paths and extraction of the data related to the retention properties is presented in Figures 6, 7 and 8.

The flow field at the repository site evolves e.g. due to the post glacial land-up lift and slow recovery of the disturbances in the salinity field caused by the open tunnels during the operational phase of the repository. In the near field of the repository the flow field can also be disturbed by the heat produced in the disposal canisters. Evolution of the site and corresponding changes in the flow conditions are represented by a series of "snapshots" in time. This approach is well applicable for the less retarded (less sorbing) nuclides, whose migration through the flow path takes place faster than the changes of the flow field. For strongly sorbing nuclides the situation is more complicated. However, bounding estimates of the transport and retention properties can be assessed for example based on the several steady state "snapshots".

It can be argued that, in a way, this approach gives a conservative estimate for the strongly sorbing nuclides. This can be reasoned in a following way. The flow field is sampled by a reasonable number of particles that are released at the canister locations. The particles that started from the same location in the repository will be spread over different locations along the flow paths as the simulation time proceeds. If the flow paths change due to the changing flow conditions at some point of time, then the particle locations along the flow paths at that time will become source locations for the flow paths of the subsequent flow field. This means that the original source used for the first flow field will become “diluted” in space for the subsequent flow fields. Steady state flow field keeps flow paths fixed and this kind of “dilution” in space does not take place.

Resolution of the element mesh may affect the calculation of the local hydrodynamic control of retention for the flow path segments. This can be tested by applying a staged procedure where the resolution of the mesh is gradually increased along the flow paths using, for example, an adaptive and iterative scheme of calculations:

1. Release particles and record the fractures that are visited by the particles.

2. Create a denser mesh over the visited fractures and a sparser mesh for the rest of the fractures.

3. Solve the flow field using the new mesh.

4. Release particles into the updated flow solution and record the flow properties along the flow paths.

5. Compare results with the outcome of the previous meshes to confirm the convergence of the results.

The mesh refinement procedure above may also be applied to take into account in-plane heterogeneity of the fractures. The flow field can first be solved for homogeneous fractures. Heterogeneity is introduced only on the fractures that are visited by the flow paths. It is possible to perform this in conjunction with the mesh refinement. However, it needs to be taken care that the effective transmissivity of the fractures do not change when the in-plane heterogeneity is introduced.

The present approach requires careful bookkeeping of the flow path segments and their properties so that the transport channels and their properties can be reproduced in the radionuclide transport calculations. The database of the flow path properties also enables robust and direct estimates of the retention using a series of simplified retention models and analytical solutions. For example, the database can be used to integrate the hydrodynamic control of retention for the entire release path and then to apply a simplistic retention model, like homogeneous and unlimited rock matrix that leads to a simple analytical estimate of the overall retention. Next step could be application of the fracture retention models in a simplified form for example to make a difference between background fractures and fracture zones.

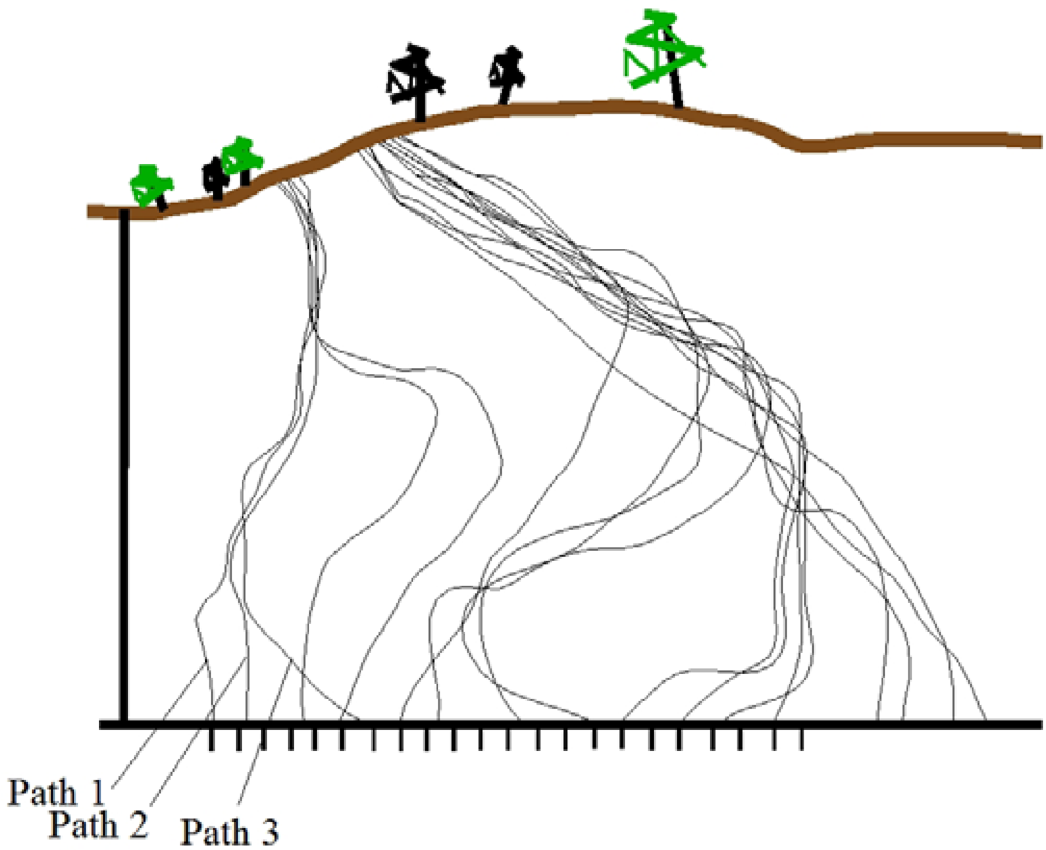


Figure 6. *Illustration of the particle tracked release paths from the repository to the surface.*

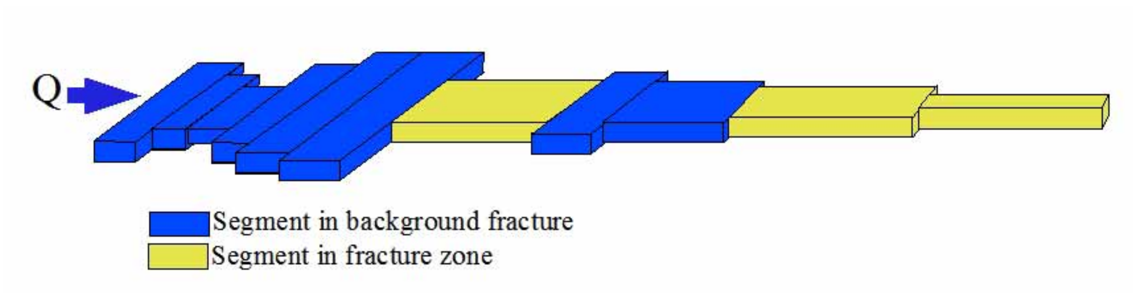


Figure 7. Flow path represented as an equivalent transport channel. Variation in the width of the equivalent transport channel indicates changes of the local flow field (i.e. WL/Q) and the colour indicates different retention models.

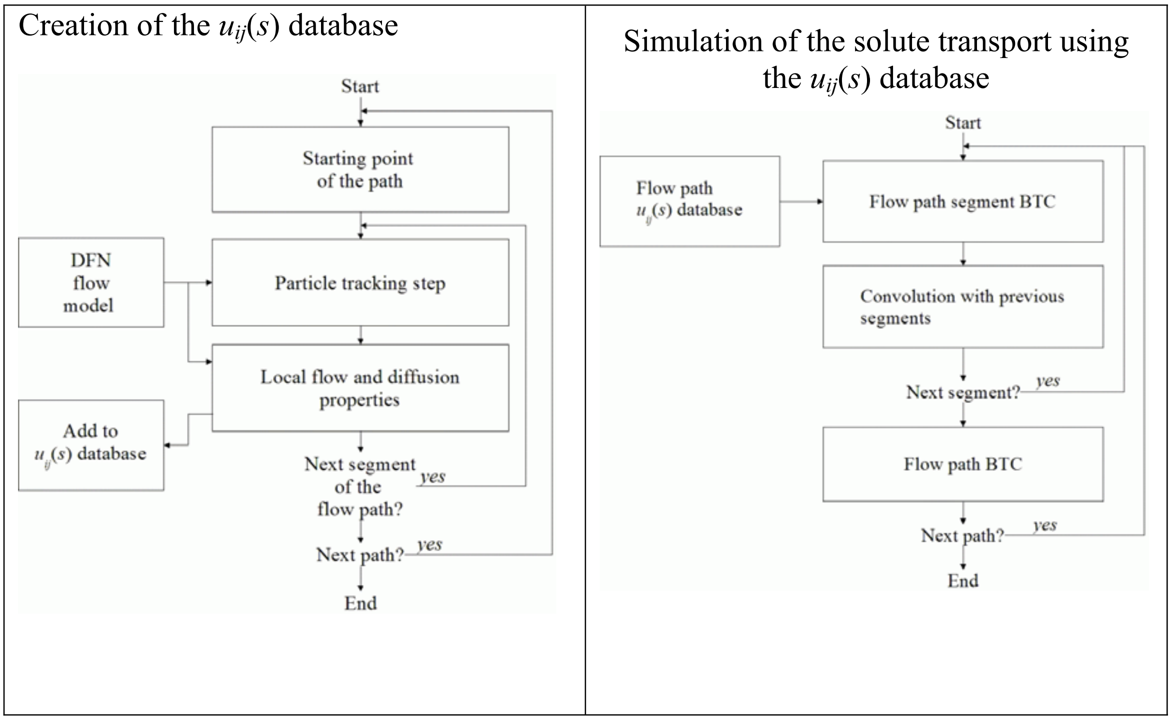


***Figure 8.** An overview of the radionuclide transport calculation scheme for the steady state analysis. The u_{ij} database refers to the Equation (22). BTC means solute breakthrough curve.*

5.3.3 Transport and retention properties along the transport channels

Transport and retention properties along the transport channels are largely controlled by the flow field. Retention along a transport channel depends on the flow rate (hydrodynamic control of retention, $\beta = 2L_j\langle W/Q\rangle_j$), immobile zone retention models and sorption properties. Geometry of the flow path determines the fractures that belong to the transport channels and, in that way, also the immobile zone retention models and sorption properties that are active in the transport channels. Transport properties are connected to the flow rates and volumes of the transport channel, which are parameterised by the transport apertures in case of the DFN model. In addition to the transport and retention properties each segment of the flow channel can be linked with other useful information like locations of the segments. The segment data for all flow paths create the database of the properties of the transport channel that is delivered to the radionuclide transport calculations (the u_{ij} database in equation (22)). Essential data on the transport channel segments is presented in the *Table 3*.

Table 3. *DFN flow model data connected to the segments of transport channels.*

Segment property	**Data type**
Hydrodynamic control retention, $L_j\langle W/Q\rangle_j$	Calculated from the local flow field
Retention model	Identification number of the model type. Coupled to the fracture type
Sorption properties	Identification number of the model type. Coupled to the fracture type or 3D location
Advective transit time	Calculated from the local flow field
Location	Calculated in the particle tracking simulation

Transport and retention properties that are calculated from the flow field are: hydrodynamic control of retention, flow path geometry (location of the segments) and advective transit time.

Locations of the transport path segments, i.e. the flow paths, are calculated using particle tracking. The accuracy and usefulness of the whole assessment of the transport and retention properties depends quite strongly on the success of the particle tracking. It does not only determine the geometry of the flow paths, but in that way it may also affect the retention properties. Success of the particle tracking depends strongly on the quality of the DFN flow solution.

Advective transit time over a segment j (i.e. j^{th} element visited along the flow path) is calculated from the local Darcy velocity, $\langle Q/W\rangle_j$, length of the pathway over the element, L_j, and fracture transport aperture, e_{t_j}, using equation $t_w = L_j\, e_{t_j} / \langle Q/W\rangle_j$.

The hydrodynamic control of retention for a segment j is estimated using the local Darcy velocity and the length of the segment in a segment-wise approximation $\beta_j = 2L_j\langle W/Q\rangle_j \approx 2L_j/\langle Q/W\rangle_j$. This approximation is reasonable if the flow field does not vary too much in the scale of the segment, and this is the case the segments are not larger than fractures.

Figure 9 elucidates estimation of the transport channels using the DFN flow model. The figure displays a piece of the particle tracked flow path by showing only the chain of the elements of the DFN flow model that are visited by the flow path. The elements are coloured to indicate the logarithm of the hydrodynamic control of retention for a unit path length ($\log10\left(1/\langle Q/W\rangle_j\right)$).

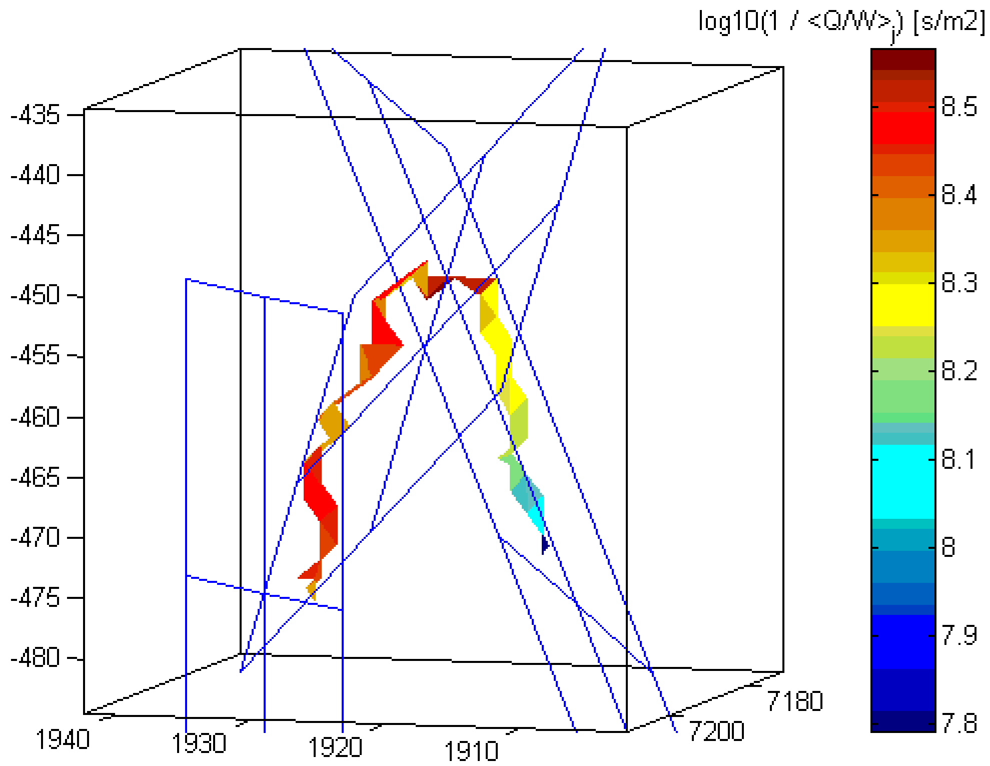


Figure 9. *An example of the particle tracked release path in the DFN model. Coloured triangles are two-dimensional elements of the numerical DFN flow model that are visited by the flow path. The colour indicates logarithm of the hydrodynamic control of retention for a unit flow path length, log10(1/<Q/W>). Fracture planes are indicated in the figure by thin blue lines.*

5.4 Transient simulations

Simulation for the snapshots in time means that the flow paths do not evolve during the course of the calculations, although the changing conditions at the site will affect also the flow paths. Transient simulations are carried out to study the influence of the changing flow geometry and flow rates to the radionuclide migration. Especially, this is significant for the strongly sorbing radionuclides that will be affected most by the gradual changes in the flow conditions, because large part of the inventory of them will be in the geosphere during the changes in the flow field.

Transport modelling needs locations of the radionuclides at the beginning of each time step. This character of the transient simulations requires that the flow field, or at least the flow paths, is solved in the same model as the radionuclide transport.

In the present concept for the transient transport calculations, based on the Marfa program, the flow field is solved by the DFN model for the specified time steps. Transport model takes the time series of the flow solutions and calculates the flow paths for each time step as the simulation proceeds.

The transient transport modelling lacks some of the transparency that there is in the steady state modelling and it is also possible that the retention models that are used in the steady state simulations are also available for the transient simulations. Steady state modelling shows explicitly an intermediate checkpoint for the flow properties along the release paths before the actual transport calculations are carried out. The transport and retention properties extracted from the flow field may also be used as direct geosphere performance measures that can help to rank and select potential deposition holes.

6 INTERFACE WITH OTHER MODELLING EFFORTS

6.1 DFN and EPM flow models

The flow model has a central role in the assessment of the transport and retention properties. The present transport concept uses a site scale DFN model as a basis of the flow modelling. DFN model is able to simulate flow distribution over different scales and it is also able to incorporate heterogeneity to the model in different scales: large deterministic features, stochastic features from local fracture zone to individual fractures and even heterogeneous fracture planes.

The transport concept does not include direct coupling to the EPM modelling. EPM modelling has an important role to build confidence and support the DFN description of the overall flow conditions. In practice, this means that both DFN and EPM flow models need to be accompanied with tools that enable model comparisons.

Assessment of the transport and retention properties is focused on the performance of the geosphere. This means that flow paths are analysed only for the portions that are along the fractures. The flow model needs to be more comprehensive in order to reproduce the flow conditions in all parts of the geosphere. Particularly this is true for the near field of the repository. The repository needs to be included to the flow model so that the flow field around the repository is more realistically described.

It can be summarized that assessment of the transport and retention properties expects following features from the DFN modelling:

- DFN model needs to be large enough to include both repository and discharge areas on the ground surface. Site scale DFN model enables simulation of the entire release paths using one model. This is also an important prerequisite for the transient radionuclide transport simulations.

- It should be easy to focus small scale details (fractures) to specified regions of the DFN model, like around the depositions holes. The volume of the site scale DFN model is going to be large, but the level of details that need to be taken into account is expected to be very different for the near field of the canisters, inside the repository and in the far-field. Flow paths follow hydraulic structures of the bedrock, which means that eventually they tend to accumulate into larger zones and small scale features can be omitted from the DFN model in the far field. Focusing detailed fracturing to specified regions can also be used to study the significance of the EDZ around the repository tunnels.

- The DFN model should be able to incorporate the in-plane heterogeneity to the fractures or part of the fractures. Heterogeneous fractures along the flow paths could be used to study influence of the channelling.

- DFN model should include engineered structures of the repository. This supports realistic simulation of the flow conditions around the repository tunnel system.

Reliable estimation of the potential release paths requires that all tunnels, deposition holes and plugs are included to the flow model. However, retention properties in the very near field of the deposition holes can be usually represented by mass transfer coefficients.

- Comparison between EPM and DFN models for the overall flow conditions should be possible. This ensures that the state of the flow conditions that has been identified by the EPM modelling is satisfactorily reproduced by the corresponding DFN model. The key properties of the flow conditions that need to be compared are the site scale flow paths and block size flow rates.

- Assessment of the transport properties requires that transport characteristics of the fractures are specified. In practice, this means specification of the transport aperture of the fractures as a part of the DFN flow model.

6.2 Geology

Majority of the data applied in the transport and retention calculations is eventually based on the geological data, for example, the DFN flow model is largely defined by the geological information on the fracturing and the DFN flow model is able to represent the site specific features of the fracturing if the coupling between DFN modelling and geology is strong enough.

Direct input from the geology to the transport and retention modelling is limited to the description of the immobile zones. Assessment of the retention properties is largely based on the retention models that should give generalised and approximate description of the rock matrix properties next to the water conducting fractures (see Section 5.2). Comprehensive application of the retention models requires that all fractures in the DFN flow model are linked with an appropriate retention model.

Retention model is not used in the DFN flow modelling and it does not affect the groundwater flow. The information is used to incorporate more accurate and site specific features of the matrix diffusion to the analysis of the transport of the radionuclides.

It can be summarized that assessment of the transport and retention properties expects from the geology:

- Specification of the retention models for the rock matrix next to the water conducting fractures and linkage of the water conducting fractures with appropriate retention models.

6.3 Geochemistry

Geochemical information is applied in the radionuclide transport calculations to give sorption properties for the radionuclides. Assessment of the transport and retention properties treats the sorption property in a very much similar way as the fracture retention models. In fact, sorption properties can be a component of the retention models. However, to retain flexibility in the radionuclide transport calculations it is better to keep the physical and chemical data separated. Physical retention models are mainly determined for the fractures or fracture types on the geological basis. Sorption properties may also be determined for subdomains of the modelling region irrespective of the local fracture types. It is also possible that sorption properties depend on the time during the expected simulation time due to the changes in the groundwater chemistry. These kinds of changes are more improbable for the physical retention models that is determined by the structure of different pore spaces.

Geochemical properties can also affect the transport and retention properties indirectly. For example, density driven flow can be notable in some regions of the model. This kind of effect is taken into account by selecting an appropriate flow model.

It can be summarized that assessment of the transport and retention properties expects from the geochemistry:

- Specification of the sorption properties for different retention models and/or different subdomains of the site-scale model. Identification and specification of a few sorption characteristics, as in the case of the retention models, are easiest to incorporate to the modelling concept. Sorption properties may also depend on time.

6.4 Biosphere

The interface between geosphere and biosphere is defined following the roles of the biosphere and geosphere modelling. Geosphere is a migration barrier that hinders the radionuclides of reaching the ground surface. Potential dose pathways are analysed as a part of the biosphere modelling. This also means that the biosphere model needs to be coupled closely with the flow model of the overburden and the upper most layer of the rock.

Assessment of the transport and retention properties expects from the biosphere modelling:

- Explicit definition of the bottom of the biosphere model to be used as upper boundary of the geosphere model

6.5 Safety case and PA

The safety case plan (Vieno and Ikonen, 2005) outlines the interface between the assessment of the transport and retention properties and actual radionuclide transport calculations. According to the plan the assessment should give estimates about the transport and retention properties and dilution in the geosphere for the next several thousand of years. It should also predict discharge areas into the biosphere to be used as an input to the biosphere assessment.

The present transport concept broadens the scope of the transport and retention calculations by the transient simulations. The base case analysis follows the safety case plan of the separate flow simulations and transport calculations. However, the model development aims to tools for the transient radionuclide transport modelling that can be used to supplement the base case analysis.

The majority of the dilution along the flow paths takes place in the top layer of the rock and in the overburden. Therefore, the geosphere flow model is not the best tool to be used for the estimation of the dilution. The main part of the diluting water does not even reach the geosphere.

The approach is to define a base case for the most realistic chain of events and parameter values. Parameter and conceptual uncertainty are studied by simplified analytical variants and conservative selection of the parameter values.

Transport and retention calculations are steered by the scenarios outlined by the performance assessment. Transport and retention modelling aim to realistic assessment of the potential geosphere retention, release paths and discharge locations to the biosphere. The key information that is used by the safety case is delivered as the geosphere performance measures. The performance measured are specified by the performance assessment and safety case and it may include for example: distribution of the flow rates in the fractures intersecting the deposition holes, distribution of the flow rates along the repository tunnels and EDZ and description of the release path properties, like path lengths, discharge locations to the biosphere and transport resistances.

Assessment of the transport and retention properties expects from the performance assessment and safety case specifications that integrate the simulations to a part of the safety case:

- Specification of the scenarios to be analysed
- Specification of the geosphere performance measures that need to be calculated

7 ILLUSTRATIVE EXAMPLES

The transport concept is applied for two examples. First, application of the equations in Section 3 is presented for a single transport channel that is in contact with an infinite rock matrix. For this case there exists a well known analytical solution. The second example illustrates assessment of the transport and retention properties for a fracture network of about 400 fractures.

It should be noted that the objective of these examples is to illustrate the concepts of the transport and retention calculations. The applied DFN data contain site specific features but the quantitative results are not specific for the Olkiluoto.

7.1 A single channel and infinite matrix

Analytical estimates of the retention are based on the equation (20). Assuming an infinite rock matrix makes it possible to calculate the Laplace transform of the diffusion term in equation (20). First, we solve Laplace transform of the equation (3) using conditions in equations (5) and (6) and requiring finite solution when z goes to infinity. The solution is (see Section 3 for definition of the parameters)

$$\tilde{g}(s,z) = \mathbf{Exp}\left(-\sqrt{\frac{s\,R_p}{D_p}}z\right) \quad . \tag{23}$$

The average diffusion flux is then

$$\left\langle \tilde{j}(s, z=0) \right\rangle = -D_e \left.\frac{\partial\,\tilde{g}(s,z)}{\partial\,z}\right|_{z=0} = D_e \sqrt{\frac{s\,Rp}{Dp}} = \sqrt{D_e R_p s} \;\; . \tag{24}$$

In this case equation (20) can be written as

$$\sum_{j=1}^{n} L_j \left\langle \frac{W}{Q} \right\rangle_j \left\langle \sqrt{D_e R_p s} \right\rangle_j \, , \qquad \sum_{j=1}^{n} L_j = L \quad . \tag{25}$$

The solute discharge in equation (19) gives

$$\frac{\tilde{\dot{m}}(L,s)}{M_0} = \mathrm{Exp}\left[-R_a\, s \frac{V}{Q} - \sqrt{s} \sum_{j=1}^{n} L_j \left\langle \frac{W}{Q} \right\rangle_j \left\langle \sqrt{D_e R_p} \right\rangle_j \right] \quad . \tag{26}$$

The Laplace transform in equation (26) can be inversed and it gives the well known solution of the solute discharge

$$\frac{\dot{m}(L,t)}{M_0} = \mathbf{H}\left(t - \frac{R_a V}{Q}\right) \frac{u}{2\sqrt{\pi}} \left(t - \frac{R_a V}{Q}\right)^{-3/2} \mathbf{Exp}\left[-\frac{u^2}{4\left(t - R_A V / Q\right)} \right], \tag{27}$$

where **H** is the Heaviside step-function and

$$u = \sum_{j=1}^{n} L_j \left\langle \frac{W}{Q} \right\rangle_j \left\langle \sqrt{D_e R_p} \right\rangle_j \quad . \tag{28}$$

7.2 Fracture network

The DFN flow model is based on three fracture sets. Each set is represented by a Fisher's orientation distribution, Power law size distribution, Log-normal transmissivity distribution and uniform fracture intensity. The model covers the whole Olkiluoto island, but it includes only the local stochastic fracture zones to avoid excessive computational needs. The minimum fracture radius has been 500 m and the maximum fracture radius has been 800 m. Deterministic large scale structures are also superimposed to the model.

Release routes are extracted from the DFN model by particle tracking. A set of 100 release locations has been randomly selected at the -410 m level around the potential repository area. *Figure 10* visualizes the calculated flow paths for both inflow paths from ground surface to the repository and release path from the repository to the ground surface. The release and inflow paths are indicated by dots along the paths. Dots are located in the centres of the visited fracture elements and the size of the dot is proportional to the number of particles that have visited it. This means that the "thickness" of the release path is proportional to the flow rate.

General view of the particle pathways shows that groundwater goes along a short pathway from the surface straight down to the repository. The release paths from the repository proceed downward until they rise to the ground surface along a major hydraulic structure.

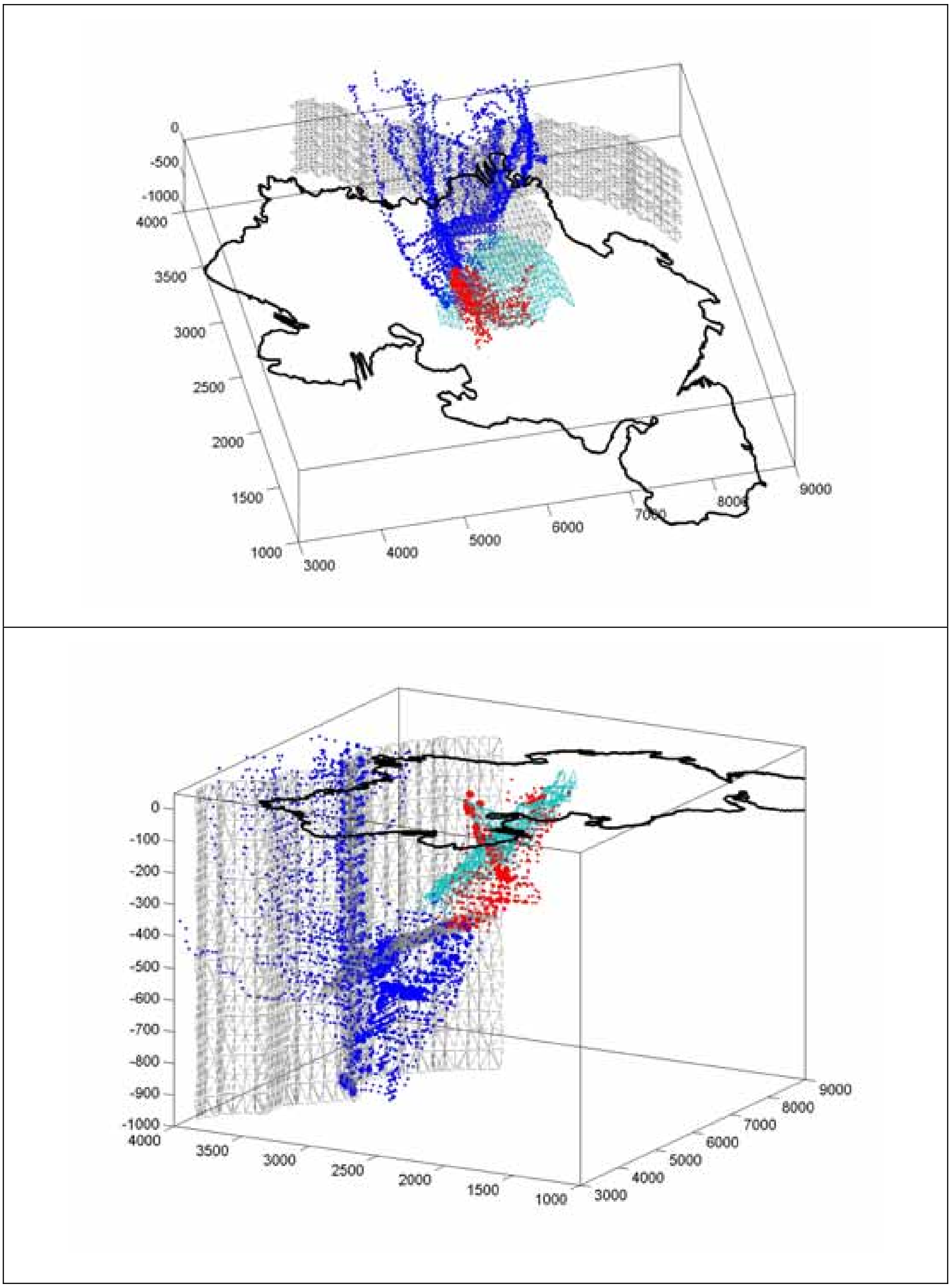
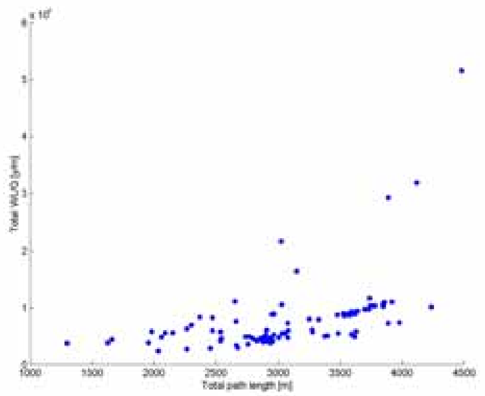


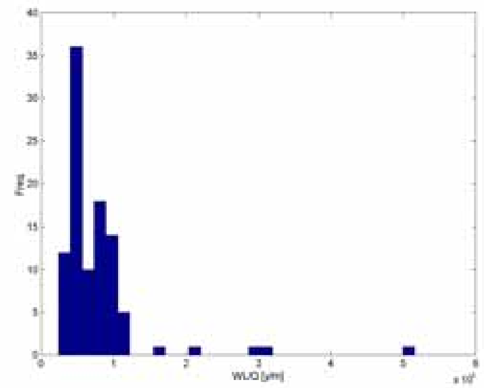
Figure 10. *Particle tracked flow paths through the DFN model. Release paths from the repository are indicated by blue dots and inflow paths from the ground surface to the repository by red dots. The sizes of the dots are proportional to the local flow rates. Some of the main hydraulic structures visited by the particles are indicated by grey lines for the release paths and by light blue lines for the inflow paths.*

Transport and retention properties for the radionuclide transport calculations are provided by the u_{ij} database (equation (22)). It is compiled from the particle tracked release paths by coupling the local flow property with the local retention model. The local flow property is approximated for each of the elements visited by the particles as $L_j\langle W/Q\rangle_j = L_j/\langle Q/W\rangle_j$, where the brackets indicate average over the element j.

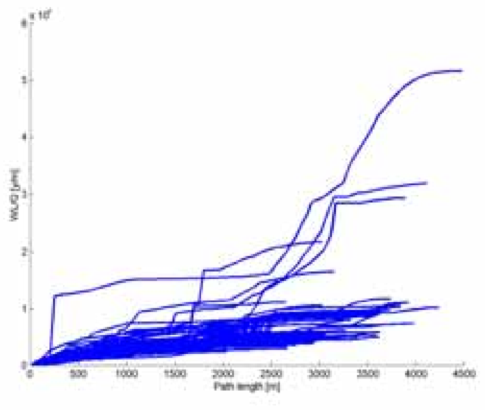
An example of the flow path statistics is presented in *Figure 11*. The present example shows rather long path lengths and advective travel times. Long travel times are explained by the large transport apertures of the fractures. Transport aperture is proportional to the square root of the transmissivity in this example. This example also shows hydrodynamic control of retention that is around $5{\cdot}10^5$ y/m that indicates significant retention. The retention is partly explained by the long flow paths.



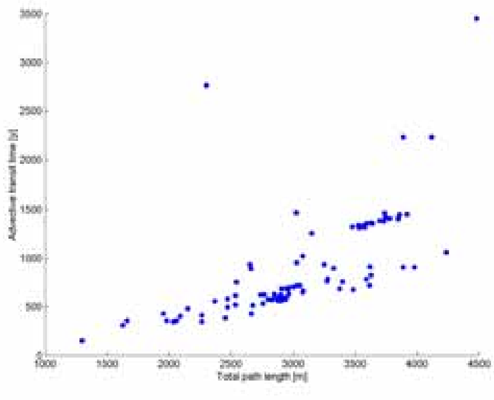
Path length vs. $\sum L_j \langle W/Q \rangle_j$



Histogram of the $\sum L_j \langle W/Q \rangle_j$



Accumulation of the $\sum L_j \langle W/Q \rangle_j$ *along the flow paths*



Path length vs. advective travel time

***Figure 11**. Statistics of the flow related transport properties along the release paths.*

Heterogeneity along the flow paths can be demonstrated by introducing retention models. Two retention models are introduced in this example. All deterministic major fracture zones are of Type 1 and stochastic fractures are of Type 2. Transport channel segments for both of the retention models are shown in *Figure 12*. The figure shows clearly that the hydrodynamic control of retention is much larger for the stochastic local fracture zones than for the larger deterministic zones.

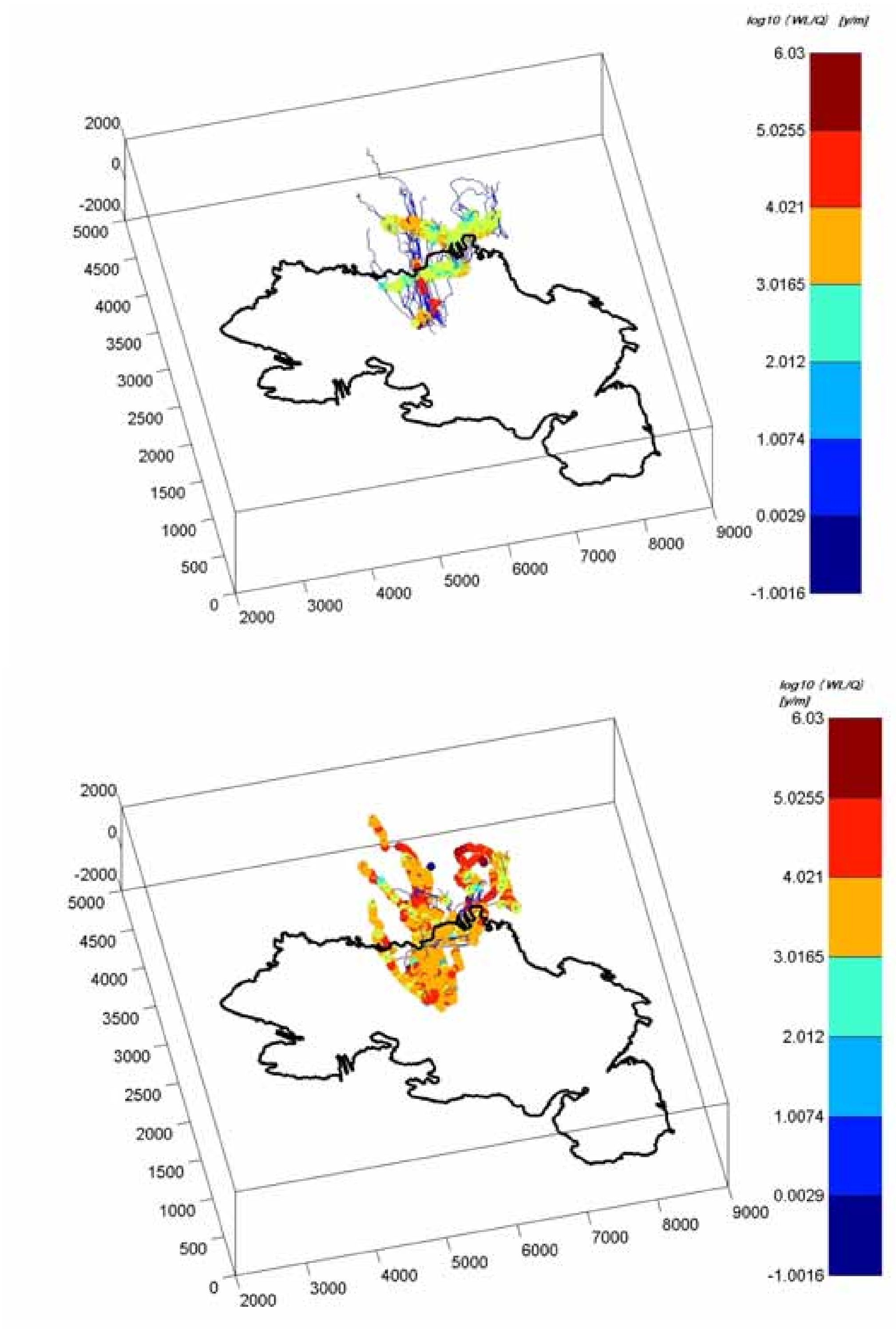


Figure 12. *Visualisation of the retention models along the release paths of the Figure 10. Release paths are indicated by the thin blue lines. Coloured dots indicate the local WL/Qs along the release paths for the Type 1 at the top (deterministic zones) and for the Type 2 at the bottom (stochastic local fracture zones).*

8 SUMMARY

This report drafts a modelling methodology that can be applied to assess transport and retention properties along flow paths in fractured rock. Simulation of the transport and retention properties for the geosphere pathways integrates data from many different sources and disciplines. Therefore, it is likely that the concept develops during the course of the site modelling and interim performance assessments and the present concept can be updated in the future when practical experience on the data collection, simulations and model interfaces is available.

Transport properties are assessed for the main geosphere retention processes: matrix diffusion and sorption. The goal is to identify properties of the flow field that are important for the geosphere retention. Data extracted from the flow model is used to characterise release paths and to derive appropriate geosphere performance measures that can be applied in the radionuclide transport calculations, performance assessment and safety case.

Characteristics of groundwater flow through fractured rock are mainly determined by structure of the rock. Great heterogeneity in the local permeability and, correspondingly, large variability of the local flow rates are typical for the fractured rock. This leads to three different characteristics of the flow: channelling that cause variable flow in the individual fracture planes, transmissivity differences between the fractures leading to preferential flow paths through the fracture network and extensive fracture zones providing highly transmissive connection over long distances. Heterogeneity is important in all scales indicating that the model size should be comparable to expected transport distances and that the flow needs to be described at the level of individual fractures, in some cases possibly even in a smaller scale determined by the channelling of the flow.

The proposed transport concept is based on application of the site scale DFN model. It is able to take into account heterogeneity in all scales. Computational feasibility can be ensured by focusing the detailed scale fracturing only to the regions of the model that have active flow paths or that are of special interest. The present transport concept takes advantage of the one dimensional nature of the solute transport through the fractured rock. In practice, this means that the transport channels are identified by particle tracking using the simulated DFN flow field. Starting locations and the number of release paths should give a statistically adequate view of the potential flow paths. Precise number of the flow paths and starting locations are agreed with the performance assessment.

The site scale flow field changes gradually due to e.g. evolution of the boundary conditions. Transport simulations need to cover a long period of time and the evolution of the flow field need also to be addressed. In the present transport and retention plan this is taken into account by building the approach on two different approaches: steady state and transient simulations.

The main part of the simulations and the approach that is also outlined in the safety case plan (Vieno and Ikonen, 2005) is based on a series of steady state simulations. In this approach radionuclide transport calculations are separated from the evaluation of the flow related transport and retention properties. Evolving flow conditions are modelled by “snapshots” in time. This methodology has many advantages: assessment of the flow conditions is not confined to any particular approach of the radionuclide transport calculations, it is easy to perform simplified analysis to bound the uncertainty analysis, conservative assumptions can be applied in a controlled way at the phase of the radionuclide transport calculations and the approach is transparent because the flow dependent component is modelled separately.

Transient modelling of the radionuclide transport in the evolving flow field requires integration of the flow and radionuclide transport models. Posiva is presently taking part to the model development that aims to transient transport modelling tool (computer program Marfa, see Appendix A). Transient simulations are applied in support of the steady state simulations.

Transport and retention simulations are focused on the flow field, but they should also provide information on the retention properties of the fractures along the flow paths. In the present transport concept this is resolved by introducing a few generalised retention models that are developed based on the site specific geological information. In practice, generalised retention models are based on the conceptualisation and parameterisation of the immobile zones next to the different types of fractures or hydraulic features. Important features of the retention model are the structure and capacity of the geological materials, like fault gouge, rock matrix alterations and unaltered rock matrix that are next to the fracture or the flow channel in the fracture. The rock matrix and geological materials are specified and quantified in respect of the main retention parameters, i.e. sorption, porosity and diffusivity.

Enhancements of the present approach compared to the previous analyses are, for example:

- Site evolution is taken into account in the flow conditions.

- Heterogeneity of the fractured rock is taken into account by explicitly including small scale fracturing into the model where it is appropriate.

- Heterogeneity of the rock mass and geological materials is taken into account by taking advantage of the generalised retention models.

- Varying sorption properties, in space or in time, can be taken into account.

Transport and retention simulations have important interfaces with DFN flow modelling, geology, geochemistry, biosphere modelling and performance assessment. DFN flow model has a central role in defining the flow characteristics, geology describes and parameterise the generalised retention models (immobile zones), geochemistry provide sorption data that connected with the retention models and biosphere modelling provides the upper model boundary of the geosphere transport and retention model. Finally, performance assessment defines calculation scenarios and performance measures for the geosphere transport paths.

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APPENDIX A: COMPUTER PROGRAMS

FEFTRA

FEFTRA is a finite element program package developed at VTT Processes for groundwater flow analyses in the site evaluation programmes. The code is capable of modelling steady-state or transient groundwater flow, solute transport and heat transfer as coupled or separate phenomena. The mathematical model consists of partial differential equations written for hydraulic head/pressure, solute concentration and temperature. The equations are coupled by means of the Darcy velocity as well as temperature and concentration dependent properties such as fluid density. When simulating solute transport, the effect of matrix diffusion can be taken into account, and highly convective cases can be handled with different upwind methods. The time discretisation in FEFTRA is based on the finite difference approximation. The matrix equations resulting from the finite element formulation can be solved either using the direct frontal solver or various iterative solvers. In coupled cases, a set of nonlinear algebraic equations is solved applying the Picard iterative approach with options for the relaxation.

The FEFTRA code uses linear or quadratic one-, two- and three-dimensional elements. Two-dimensional elements can also be applied in a three-dimensional mesh and one-dimensional elements in both two and three-dimensional meshes. For example, in three-dimensional groundwater flow simulations, sparsely fractured rock can be described by three-dimensional elements, fracture zones or other planar structures by two-dimensional elements and tunnels by one-dimensional elements. An advanced preprocessor includes, e.g., quadtree/octree algorithm, which enables an efficient local refinement of mesh around natural and engineered bedrock structures (e.g. fracture zones, sinks, tunnels, etc.) (static mode) or at the locations with high hydraulic gradient (dynamic mode).

Ref.:

VINTAGE (Virtual Integer Arithmetics to Generate Elements)

Simulations involving discrete fracture networks (DFNs) are often based on a stochastic approach, which involves several realisations of the model from the same statistical parameters that describe the DFN. The principal steps of this approach are

- generating the DFN
- discretisation, i.e. converting the fracture geometry to finite elements
- assigning properties, prescribing boundary conditions
- solving the model
- postprocessing the results.

for all realisations. A significant bottleneck in this process turned out to be the discretisation phase, which, performed with any existing tools, proved computationally at least as expensive as the solution itself. The algorithm implemented in the new tool was specifically developed to address this problem. Considering that integer calculations are significantly faster than those involving floating point numbers, the basic idea of this approach was to re-map the DFN geometry into integer space and perform the discretisation there, only using integer arithmetics. The very core of the algorithm produces the finite element mesh fast enough that all the phases of the simulation combined that precede the solution of the model are carried out within an order of magnitude less time than the solution phase, thus constituting no bottleneck of the simulation any longer.

The VINTAGE code (the DFN module of the FEFTRA program package) has been tested with real data characterising the Olkiluoto site.

Postprocessing the calculated head field with a particle tracking algorithm predicts the flow paths' geometry between the boundary conditions, the travel times and the flow resistance WL/Q quantities.

Ref.: Program is under development

MARFA

The computer code MARFA (Migration Analysis for Radionuclides in the FAr field) uses a particle-based Monte Carlo method to simulate the transport of radionuclides in a sparsely fractured geological barrier. The particle on random streamline segment algorithm combines time domain random walks with pathway stochastic simulation. Radionuclide mass is represented by non-interacting particles that are moved through the system according to rules that mimic the underlying physical transport and retention processes. Transport and retention properties are limited to those that depend linearly on radionuclide concentration. Non-linear processes such as solubility-limited transport or aqueous speciation are not represented.

The MARFA code is specifically designed to work with output from discrete fracture network (DFN), continuous porous medium (CPM) or nested DFN/CMP flow models. The physical processes represented in MARFA include advection, longitudinal dispersion, diffusion into an infinite or finite rock matrix, equilibrium sorption, decay and in-growth. Multiple non-branching decay chains of arbitrary length are supported.

Ref.: MARFA Version 3.1β user's manual: Migration analysis of radionuclides in the far field. Program is under development.

ConnectFlow

CONNECTFLOW is the suite of Serco Assurance's groundwater modelling software that includes the NAMMU continuum porous medium (CPM) module and the NAPSAC discrete fracture network (DFN) module. CONNECTFLOW is also the name given to the concept of nesting NAMMU and NAPSAC sub-models into a combined CPM/DFN model. CONNECTFLOW is very flexible tool for modelling groundwater flow and transport in both fractured and porous media on a variety of scales.

CONNECTFLOW has been developed by Serco Assurance (formally AEA Technology) over the last 10 years. It is developed under a rigorous quality system that conforms to the international standards ISO 9001 and TickIT. CONNECTFLOW can be used to model the following physics and geometries:

- 3D models;
- single or multiple DFN sub-regions nested within CPM regions;
- single CPM sub-regions nested within DFN region;
- stratigraphic layers with DFN representation can be interfaced to layers with a CPM representation;
- models are built up of grids with different patches being assigned to either a CPM or DFN subdomain;
- nesting of detailed DFN models within nested CPM models using embedded ('constraint') grids to represent site-scale and region-scales;
- stochastic DFN and CPM models;
- steady-state and transient constant-density groundwater flow;
- advective transport through a combined DFN/CPM based on a particle tracking approach.

CONNECTFLOW can be used to model the following features:

- local DFN models to represent the detailed flow in fractures around tunnels, shafts, canisters or boreholes nested within a CPM model that extends the model to appropriate boundaries;
- detailed CPM models of tunnels, shafts and canisters within a DFN model to represent the interaction between flow in a fractured media and backfilled tunnels;
- continuous representation of deterministic faults/fracture zones through the DFN and CPM sub-models using consistent data formats and a combination of explicit fracture planes in DFN regions and an implicit fracture zone (IFZ) method in the CPM region.
- quantifying conceptual uncertainties between DFN and CPM models.

Using the CONNECTFLOW suite of programs allows the development of integrated groundwater flow and transport models using the combined concepts of discrete fracture networks and continuum modelling without the need to export boundary conditions from one model to another.

Ref.: www.connectflow.com

FTRANS (Fractured Flow and Transport of Radio-Nuclides)

FTRANS is a two-dimensional FEM code that can simulate groundwater flow and transport of radioactive decay chains in porous and fractures media. It can be acquired from OECD/NEA Data Bank. The migration part of FTRANS can handle convection, dispersion, retardation based on the equilibrium sorption both on fracture surface and in rock matrix, matrix diffusion, and radioactive chain decay. The code offers unusual flexibility in describing initial and boundary conditions. Time integration in FTRANS is based on two optional finite difference methods: either Crank-Nicolson or fully implicit backward difference schemes.

Ref.: INTERA Environmental Consultants, Inc., FTRANS: A two-dimensional code for simulating fluid flow and transport of radioactive nuclides in fractured rock for repository performance assessment, 1983, Technical Report ONWI-426.