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Assessment model validity document FARF31

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Abstract

The prime goal of model validation is to build confidence in the model concept and that the model is fit for its intended purpose. In other words:

- Does the model predict transport in fractured rock adequately to be used in repository performance assessments?
- Are the results reasonable for the type of modelling tasks the model is designed for?

Commonly, in performance assessments a large number of realisations of flow and transport is made to cover the associated uncertainties. Thus, the flow and transport including radioactive chain decay are preferably calculated in the same model framework. A rather sophisticated concept is necessary to be able to model flow and radionuclide transport in the near field and far field of a deep repository, also including radioactive chain decay. In order to avoid excessively long computational times there is a need for well-based simplifications. For this reason, the far field code FARF31 is made relatively simple, and calculates transport by using averaged entities to represent the most important processes.

FARF31 has been shown to be suitable for the performance assessments within the SKB studies, e.g. SR 97. Among the advantages are that it is a fast, simple and robust code, which enables handling of many realisations with wide spread in parameters in combination with chain decay of radionuclides. Being a component in the model chain PROPER, it is easy to assign statistical distributions to the input parameters. Due to the formulation of the advection-dispersion equation in FARF31 it is possible to perform the groundwater flow calculations separately.

The basis for the modelling is a stream tube, i.e. a volume of rock including fractures with flowing water, with the walls of the imaginary stream tube defined by streamlines. The transport within the stream tube is described using a dual porosity continuum approach, where it is assumed that rock can be divided into two distinct domains with different types of porosity – fractures with flowing water and rock with porosity accessible only by diffusion. The approach furthermore assumes that the properties within the two porosity domains are averaged and also the transfer between the two domains is averaged.

It is an important validation issue to verify that effective averaging of parameters can be performed and that suitable values can be derived. It can be shown that matrix interaction properties along a flow path can be integrated to an effective value and if the matrix depth can be considered as infinite, effective values may be derived also for the diffusion and sorption parameters. Thus, it is possible to derive effective parameters for sorbing radionuclides incorporating the total matrix effects along a flow path. This is strictly valid only for cases with no dispersion, but gives a good approximation as long as dispersion does not dominate the transport.

FARF31 has been tested and compared with analytical solutions and other models and was found to correspond well within a wide range of input parameters. Support and documentation on how to use FARF31 are two important components to avoid calculation mistakes and obtain trustworthy results. The documentation describes handling and updates of the code. Test cases have been constructed which can be used to check updates and be used as templates. The development of the code is kept under source code control to fulfil quality assurance. The model is deemed to be well suited for performance assessments within the SKB framework.

Sammanfattning

Huvudmålet med modellvalidering är att bygga förtroende för modellkonceptet och att modellen passar för sin användning. Med andra ord:

- Predikterar modellen transport i sprickigt berg på ett adekvat sätt för att användas vid säkerhetsanalys av ett förvar?
- Är resultaten rimliga för den typ av modellering som modellen är designad för?

I en säkerhetsanalys görs vanligen ett stort antal realiseringar av flöde och transport för att täcka in osäkerheter i systemet. Därför beräknas flöde och transport inklusive radioaktivt sönderfall företrädesvis med samma modellpaket. Ett tämligen sofistikerat modellkoncept är nödvändigt för att kunna modellera flöde och radionuklidtransport i närzon och fjärrzon, även inkluderande radioaktivt kedjesönderfall. För att undvika orimligt långa beräkningstider finns ett behov av välgrundade förenklingar. Av denna anledning har fjärrzonskoden FARF31 gjorts relativt enkel och beräknar transporten med hjälp av medelvärdesbildade enheter för att representera de viktigaste processerna.

FARF31 har visat sig lämplig till SKB:s säkerhetsanalyser, t ex SR 97. Bland fördelarna är att den är snabb, enkel och robust, vilket möjliggör hantering av många realiseringar med en stor spridning på parametervärdena i kombination med radioaktivt kedjesönderfall. Som en komponent i modellkedjan PROPER är det lätt att tilldela statistiska fördelningar till indataparametrarna. Formuleringen av advektions-dispersionsekvationen i FARF31 gör det möjligt att utföra grundvattenflödesberäkningarna separat.

Grunden för modellen är ett strömrör, dvs en bergvolym inkluderande vattenförande sprickor där väggarna ges av strömlinjer. Transporten i strömröret beskrivs med hjälp av antagande om ett kontinuum med dubbelporositet, “dual porosity continuum”, där berget antas kunna delas in i två distinkta domäner med olika typ av porositet – vattenförande sprickor respektive berg med en porositet som endast är tillgänglig genom diffusion. Detta angreppssätt antar vidare att medelvärdesbildning kan göras för egenskaperna inom de olika domänerna samt även för överföringen mellan domänerna.

Eftersom berget och sprickornas egenskaper i strömröret medelvärdesbildas över hela dess längd är det viktigt ur valideringshänseende att kunna göra en effektiv medelvärdesbildning av parametrarna och att passande värden kan tas fram. Det kan visas att matrisens interaktionsegenskaper längs flödesvägen kan integreras till ett effektivt värde och om matrisens djup kan antas vara oändligt kan effektiva värden erhållas även för diffusions- och sorptionsparametrar. Således är det möjligt att ta fram effektiva parametrar för sorberande radionuklider som inkluderar den totala effekten av matrisen längs flödesvägen. Denna approximation är strikt endast giltig för fall utan dispersion, men ger en god approximation så länge dispersionen inte dominerar transporten.

FARF31 har testats och jämförts med analytiska lösningar och andra modeller med god överensstämmelse över ett stort intervall på indataparametrarna. Support och dokumentation av hur FARF31 används är två viktiga komponenter för att undvika beräkningsmisstag och erhålla trovärdiga resultat. Dokumentationen beskriver användning och uppdatering av koden. Testfall har satts upp och kan användas som mallar och för att kontrollera uppdateringar. Utvecklingen av koden registreras i ett versionskontrollsystem för att uppfylla kvalitetskraven. Modellen bedöms vara väl lämpad för SKB:s säkerhetsanalyser.

Contents

1 Introduction

The model FARF31 /Norman and Kjellbert, 1990/ calculates the transport of dissolved radionuclides through the fractured rock, the retention caused by interactions between the nuclides and the rock matrix, and the radioactive chain decay. The processes included are:

- *advection* – transport of radionuclides by water flowing through fractures in the rock,
- *dispersion* – the spreading caused by velocity variations between different fractures or in different parts of a fracture,
- *matrix diffusion and sorption* – the diffusive transport of radionuclides from the water in the fracture into pores and microfissures of the rock matrix where the nuclides may sorb on the solid surfaces,
- *radioactive decay and chain decay*– the decay of individual radionuclides and the decay and in-growth of radionuclides that are members of a decay chain.

The far-field code FARF31 calculates radionuclide transport using a stream tube concept. It has been developed to be a tool to aid performance assessments of repositories for radioactive waste. For example, FARF31 has been used for radionuclide transport calculations in the performance assessments SKB 91 and SR 97. Commonly, FARF31 takes input data from a groundwater flow model and a near-field model. In SKB 91, groundwater travel times for 88 stream tubes distributed over the repository area were calculated in HYDRASTAR, and used as part of the input data to FARF31. A similar concept was used in SR 97 to calculate radionuclide transport for three sites. It is possible to use FARF31 stand-alone or as a component in the model chain within the PROPER package enabling probabilistic simulations.

Similar to validation documents written for other model concepts, such as NAMMU /Cliffe et al, 1998/, COMP23 /Romero et al, 1995/ and HYDRASTAR /Gylling and Eriksson, 2001/, validation is here defined as a process of building confidence in the calculation tool. Comparing calculation results with measured values from field experiments is probably the most important issue in the validation process. Since data from field experiments are scarce, especially for the type of problem FARF31 is designed for, other sources can also be used to build confidence in the model concept. One method is to compare results with the ones achieved using other model concepts for the same set of input data. Comparison with analytical solutions is another way to check that the model is doing what it is designed for. The latter is often included in the process of verification, i.e. checking that the used numerical method is handling the underlying mathematical equations correctly. Support and documentation on how to use such an expert code as FARF31 are two important components to avoid calculation mistakes and obtain trustworthy results. In addition to document and to handle developments, the use of a source code control system is required to fulfil quality assurance.

1.1 FARF31 in the PROPER framework

The main use of FARF31 is as a submodel within the PROPER package. PROPER (PRObabilistic PERformance-assessment) is a modularised code package where the submodels describe different aspects of the radionuclide transport. The main submodels today are:

- HYDR11 (or HYDRASTAR) an integrated finite difference groundwater flow model. Presently, other groundwater flow models, not included in the PROPER package are frequently used, for example CONNECTFLOW or DarcyTools.
- COMP23 a near-field transport model using a very coarsely discretised integrated finite difference model and embedded analytical solutions at sensitive zones.
- FARF31 a far-field transport model.
- BIO42 a dose conversion model.

PROPER administrates the input, controls the execution of the computations in each module and collects the crude statistics.

The input to FARF31 comprises both parameters that are possible to assign statistical distributions, constant parameters and input time series, see Figure 1-1. PROPER handles the choice of parameter values for the present realisation and administrates the transfer of the groundwater travel times from the groundwater flow model to FARF31 and output time series from the near-field model to FARF31 as input time series. The output time series from FARF31 are possible to transfer for further calculations in BIO42. In BIO42 the far-field release rates are possible to sum and/or to convert to dose by multiplication with precalculated dose conversion factors.

Outputs from FARF31 are mainly the output time series, including the radionuclide release rates (Bq/year) as a function of time. The possibility of collecting crude statistics in PROPER may for example be used to collect maximum release rates from the far field for each radionuclide.

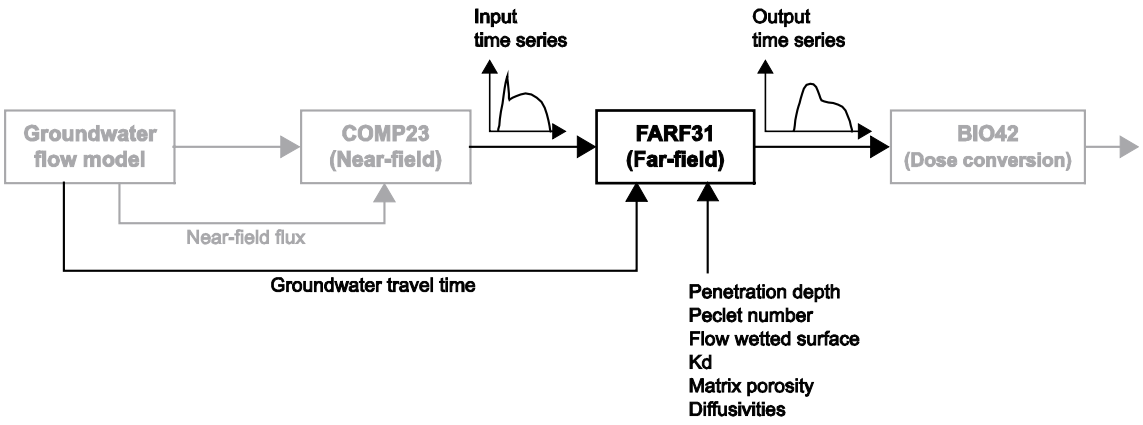

Figure 1-1. *Schematic illustration of the input and output of time series and parameters to and from FARF31.*

In the recent safety analysis SR 97, a scenario including an initially defect canister was analysed for three hypothetical sites (Aberg, Beberg and Ceberg). Several deterministic calculations were made as well as probabilistic calculations including a large number of realisations to cover the effect of uncertainty. In SR 97 the model package PROPER including FARF31 was used. The groundwater travel times were calculated with HYDRASTAR for 100 realisations each containing 120 stream tubes distributed over the repository area. The results from HYDRASTAR were saved for later use in PROPER.

In the PROPER simulations 5000 realisations were performed for the near field, far field and dose conversion. The initial canister defect was simulated by assigning a probability of 0.9 that a single canister is initially defect and a probability of 0.1 that five canisters are defect. This results in one or five sets of COMP23 and FARF31 in parallel. As input to FARF31 the groundwater travel times for stream tubes originating from positions of failed canisters (one or five) were chosen among 120 stream tubes representing the repository area. Most of the other input parameters were assigned a probability of 0.9 of having a reasonable parameter value and a probability of 0.1 of having a pessimistic value. This concerns the parameters flow wetted surface, radionuclide specific K_d and radionuclide specific diffusivities. The porosity, penetration depth and Peclet number were always assigned pessimistic values, due to limitations in the FARF31 version used in SR 97.

2 Conceptual model

In Sweden as in many other countries, it is planned to dispose of spent nuclear fuel in crystalline rock at depth. In the repository for nuclear waste, the canisters containing the waste will be surrounded by low conducting clay, bentonite. The canisters are designed such that the canister will have a very long lifetime in the repository environment. When the canisters eventually degrade after a long time, or in the case of an initially defect canister, the nuclides may diffuse through the clay and eventually reach the crystalline rock. In fractures in the rock, there can be a flow of water that can transport the nuclides. However, the water flow rates at suitable repository locations are expected to be low and retardation mechanisms will slow down the transport.

Because of the possibility of radionuclides escaping the repository, performance assessment are needed to test the design and construction of the repository. In the performance assessment, modelling of water flow and solute transport is an important tool. Commonly, in the performance assessment the case of an initial damage of the canister is considered.

2.1 Flow and transport in fractured rock

In the rock, water may flow in fractures and fracture zones that lead to a very heterogeneous flow distribution. This has been observed in boreholes and in tunnels and drifts at e.g. Stripa, Finnsjön, Grimsel and Äspö. The uneven flow distribution is due to that the water will seek out the easiest paths for the prevailing gradient and may cause a portion of the solutes to travel relatively fast compared to the remaining portion, i.e. channeling. Released solutes may thus become spread. The flow paths may intersect in the geosphere, so that a network of paths is formed. At the path intersections there may be mixing of the waters originating from different flow paths.

At the same time, different interaction mechanisms may retard the transport of the solutes. Figure 2-1 shows an illustration of the interaction mechanisms. The main interaction mechanisms are diffusion of the solutes into the rock matrix and sorption /Birgersson and Neretnieks, 1990/. This results in delay of the release and thereby increased time for the decay of radioactive nuclides. The interaction between the solutes and the rock takes place at the available interaction surface (flow-wetted surface area). The quotient of the flow-wetted surface area to the flow rate is one of the key entities /Neretnieks, 1980; Moreno and Neretnieks, 1993/. The geometry of the flow path and the flow distribution are thus of major importance for the rock interaction.

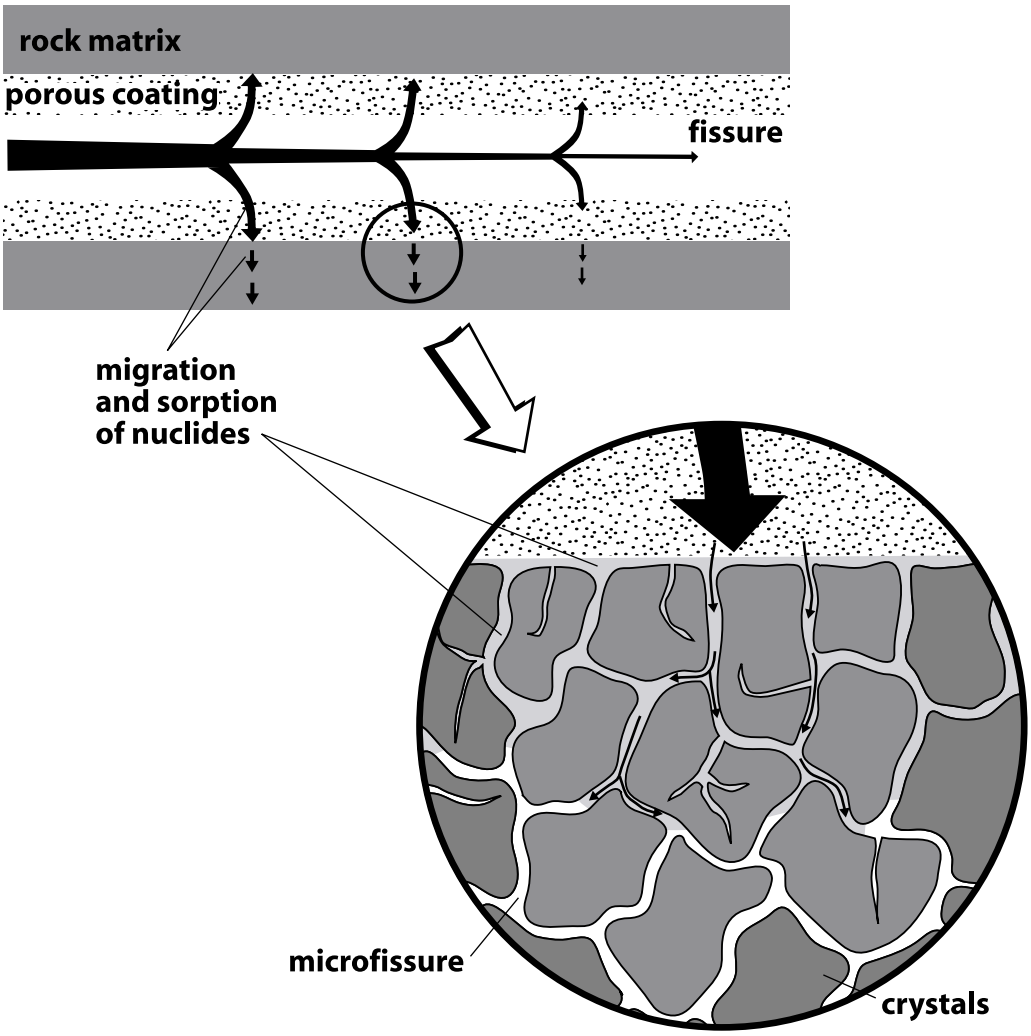

Figure 2-1. *Matrix diffusion and sorption in the microfissures in the rock matrix /Redrawn from Neretnieks, 1993/.*

2.1.1 Matrix diffusion

As the solutes are transported by advection they have the ability to diffuse into the stagnant water in the microfractures in the rock, which is of great importance as the matrix diffusion provides a possibility of sorption on the relatively large surface area within the rock matrix. If the direction of the concentration gradient is the opposite e.g. after a pulse of radionuclides passed in the fracture, solutes may diffuse back into the flowing water. The transfer rate into the matrix depends on the effective diffusivity and the concentration gradient. Diffusivity depends both on the geological material and the type of radionuclide concerned. Rock types have different porosity and pore structure that affects their diffusivity. Measurements have also shown that the parts of the rock adjacent to fractures have an increased porosity /Valkiainen, 1992; Landström et al, 2001/ giving an increased effective diffusivity.

The dependency of type of radionuclide is relatively weak. Most cations have similar diffusivities.

Since the gradient in the pore water decreases as more solute diffuses into the matrix so will also the transfer rate. Thus, the rate of transfer over time depends on the sorptive properties of the radionuclide. The penetration depth also depends on the diffusivity and the sorptive

properties, but the maximum penetration depth may be controlled by geometric factors such as extent of porous layers or distance to other water bearing fractures.

In water with low ionic strength, anions have a lower diffusivity into the matrix compared to uncharged solutes with otherwise identical properties. This anion exclusion effect is due to the repulsion between the normally negatively charged rock material and the anions, which gives a smaller effective volume available for diffusion /Ohlsson and Neretnieks, 1997/. Diffusion of cations that undergo ion exchange can be reinforced by surface sorption. In this case the radionuclides diffuse on the surface of the solid phase as well /Skagius, 1986/.

2.1.2 Sorption

Sorption, where radionuclides sorb to the surfaces of the fracture system and the rock matrix, is important for radionuclide transport. Sorption on the interior of the rock matrix is considered to be more important than on the fracture surfaces, since there is far more surface area available in the matrix compared to the area of the fracture surfaces. The term sorption embraces a number of different retention processes and mechanisms that result in the adherence of radionuclides on the rock surfaces or on other material that may be present on the fracture surfaces. The strength of sorption depends on the chemical properties of the rock, the solute (radionuclide) and the chemical conditions, e.g. salinity and the presence of complexing agents. Some solutes may not sorb or the sorption can be negligible, but may still be delayed by matrix diffusion into the additional pore space of the rock.

A large number of experimental, nuclide-specific studies of sorption have been conducted /cf Carbol and Engkvist, 1997/. In modelling, sorption is commonly expressed by a distribution coefficient, K_d. If the sorption is linear, reversible and at equilibrium, a K_d value can be estimated for the particular water composition. The assumption of linearity is usually fulfilled at the low concentrations that are of interest, while the assumption of equilibrium is fulfilled if the sorption is substantially faster than the transport by advection and dispersion. If the solute has diffused into the matrix more time is available for sorption. The rock type is also influencing K_d, but for Swedish crystalline rocks similar values have been reported /SKB, 1999/. Salinity has, however, a great impact on the K_d-value.

2.2 Basic assumptions

The basis for the modelling is a stream tube, i.e. a volume of rock including fractures with flowing water. The walls of the imaginary stream tube are defined by streamlines. As a consequence, no water is allowed to pass through walls of the stream tube and thus all mass entering one end of a stream tube will subsequently be discharged at the other end. FARF31 does not explicitly consider the transport in individual fractures and flow paths contained within the stream tube. Instead, the transport properties of the water-bearing fractures and the rock matrix available through diffusion are averaged over the stream tube, using the dual porosity continuum approach. The stream tube concept greatly facilitates the radionuclide transport modelling. The complex three-dimensional flow field is thus divided into a set of one-dimensional stream tubes.

In the dual porosity approach it is assumed that rock can be divided into two distinct domains with different types of porosity – fractures with flowing water and rock with porosity accessible only by diffusion. The approach furthermore assumes that the properties of the two porosity domains are averaged and also the transfer between the two domains is averaged.

2.3 Treatment of transport and retention processes

Only a small portion of the volume of the rock is taken up by cavities such as fractures and porous structures in the intact rock. The groundwater flows in these cavities, but only through fractures that are hydraulically connected and through that portion of the fracture volume that is open to flow. The flow porosity, which is smaller than the total porosity of the rock, is the portion of the rock that is taken up by flowing groundwater. The total groundwater flow per unit area is called the Darcy velocity. The mean transport velocity of the water particles is obtained as the Darcy velocity divided by the flow porosity. This resultant transport process of solutes in the groundwater is called advection.

The Darcy velocity is defined on a macroscopic scale. On smaller scales, velocity differences occur for the flow within a fracture and between different fractures. These velocity variations lead to mixing phenomena called hydrodynamic dispersion. During transport in fractured rock, the dispersion is usually dominated by velocity variations between different flow paths.

The division of transport into an advective and a dispersive component is dependent on the scale studied and is relatively arbitrary. The advective component describes the mean transport, while the dispersive component takes into account velocity variations caused by the heterogeneity in the rock at smaller scales than what is described by the advective component. Dispersion is a model concept rather than an actual process Dispersion is often assumed to increase linearly with the water velocity. Dispersion also contains a component that describes pure molecular diffusion in water. The dispersivity is often defined as:

$$D_L = \alpha\, u_0 + D_e$$

where:

α is the dispersion length
u_0 is the Darcy velocity
D_e is the effective molecular diffusivity.

The first term gives the contribution due to hydrodynamic dispersion and the second term the contribution due to molecular diffusion.

The combined effect of advection and dispersion can be described by the advection-dispersion equation:

$$R_a \frac{\partial C}{\partial t} = D_L \frac{\partial^2 C}{\partial x^2} - u_0 \frac{\partial C}{\partial x}$$

where:

R_a is the surface retardation factor, $R_a = \varepsilon_f + K_a \cdot a_w \cdot \varepsilon_f$
ε_f is the flow porosity
K_a is the surface sorption coefficient (1/m)
a_w is the flow wetted surface per volume of water (m^2/m^3)
C is the concentration
x is the transport distance.

Transport by molecular diffusion takes place when solutes move from areas of high concentration to areas of low concentration. Molecular diffusion is primarily important in conjunction with matrix diffusion in the rock's water-filled microfractures. Molecular diffusion in the flowing water is generally negligible compared to the effect of advection and dispersion. However, the process can be of importance for transport of radionuclides into zones of stagnant water in fractures.

In case of one-dimensional problems, the mass flux due to the pore water diffusion can be expressed as:

$$J_p = -D_e \frac{\partial C}{\partial x}$$

The change in concentration at a given point with time may be expressed by Fick's second law:

$$R \frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2}$$

Solutions to this equation with appropriate initial and boundary condition give the concentration as a function of time and space.

The relationship between the concentration of a sorbed and dissolved radionuclide may be described by a sorption isotherm. Several alternative formulations for the sorption isotherm exist, e.g. the Langmuir or the Freundlich isotherm. In FARF31 the assumption of linear equilibrium sorption, the so-called K_d-concept, is used. This implies that the sorption reactions are fast compared to the transport processes and that there is a linear relationship between the concentration of sorbed and dissolved radionuclide given by:

$$C_s = K_d \cdot C_p$$

where:

C_s is the concentration of sorbed radionuclide
C_p is the concentration of radionuclide in pore water.

The use of a K_d-value to describe sorption greatly simplifies the mathematical treatment of coupled sorption and transport. For low concentrations of the radionuclide, the potential error introduced by assuming linear sorption is generally small compared to the uncertainty in the available sorption data.

With the assumption of linear sorption, a retardation factor can be defined which gives the ratio between the travel time for a sorbing species to that of a non-sorbing species. The retardation factor is given by:

$$R = \varepsilon + K_d \rho$$

where:

ε is the matrix porosity
K_d is the distribution coefficient of the sorbing species
ρ is the bulk density of the rock.

Flow-averaging

FARF31 is based on the one-dimensional advection-dispersion equation with one-dimensional diffusion perpendicular to the flow into a matrix of finite depth. The equation is formulated in flux averaged quantities of concentration, water velocity, dispersivity and the exchange rate between flowing water and the pores of the rock matrix. The distance in the flow direction is transformed into accumulated groundwater travel time. Thus, the parameters determining the advection-dispersion are the groundwater travel time (t_w) and the Peclet number (Pe). This allowing for the use of groundwater travel times computed externally (by HYDRASTAR or by some other groundwater flow code). The retention mechanism considered by FARF31 is the diffusion of radionuclides into the rock matrix where they may sorb on the inner surface of the rock. Sorption directly on the fracture surface is not included.

Since the rock volume encompassed by a stream tube will contain many flow paths, it is useful to employ the concept of specific flow-wetted surface, e.g. by defining the contact area between the flowing water and the fracture surfaces per unit volume of flowing water (a_w). Retention of radionuclides in fractured rock has been found to depend strongly on the ratio between the flow-wetted surface and the water-flow rate. This may be taken into account in FARF31 by using the F-factor, which can be expressed as the product of the groundwater travel time and the flow-wetted surface per volume of water in the transport pathway ($t_w \cdot a_w$). One should note, however, that t_w is essentially proportional to the flow porosity whereas a_w is essentially inversely proportional to the flow porosity, making the product $t_w \cdot a_w$ almost insensitive to the flow porosity /Andersson et al, 1998/. Consequently, the F-factor is not directly dependent on the groundwater travel time but rather the groundwater flux and on the geometrical distribution of the flow in the fractures.

In order to describe matrix diffusion and sorption, data is required for effective matrix diffusivity (D_e), matrix porosity (ε), maximum penetration depth (x_0) and distribution coefficients for the different radionuclides (K_d). A new version of FARF31 that includes the capability of using element specific values for the matrix diffusivity was developed within SR 97 /Eriksson et al, 1999/.

3 Mathematical formulation and solution techniques

FARF31 is based on the one-dimensional advection-dispersion equation with one-dimensional diffusion into a matrix of finite depth. Furthermore, radioactive chain decay is included.

3.1 Mathematical formulation

In FARF31 the transport equations assuming a Dirac pulse input are solved analytically in the Laplace domain. The solution is numerically inverted to the real time domain to obtain a response function. This function is convoluted with the actual inlet flow to the stream tube to obtain the outlet flow.

The following assumptions form the basis for the underlying equations:

(i) stationary flow conditions prevail,

(ii) transversal dispersion may be neglected,

(iii) the longitudinal dispersion coefficient and the exchange terms between flow- and diffusional porosity may be replaced by averages over the stream tube cross section,

(iv) the density is constant and the variation of porosity is small compared to the variation of concentration,

(v) the stream tube is sufficiently narrow to warrant the assumption that the pore velocity may be replaced by some average over the cross section and

(vi) only non-branched decay chains can be used.

The equations on which FARF31 is based are in summary:

$$\frac{\partial c_i}{\partial t} = -\frac{\partial c_i}{\partial \zeta} + \frac{t_w}{Pe}\frac{\partial^2 c_i}{\partial \zeta^2} + a_w D_e \left.\frac{\partial c_i}{\partial x}\right|_{x=0} - \lambda_i c_i + \lambda_{i-1} c_{i-1}$$

$$R_i \frac{\partial c_{p,i}}{\partial t} = D_e \frac{\partial^2 c_{p,i}}{\partial x^2} - R_i \lambda_i c_{p,i} + R_{i-1} \lambda_{i-1} c_{p,i-1}$$

where:

c_i is the flux-averaged concentration in the flowing water
$c_{p,i}$ is the surface and flux-averaged concentration of radionuclide i in the pore water
t_w is the groundwater travel time in the flowing water
t is the time
a_w is the flow-wetted surface per volume of water

ζ is the distance in the flow direction expressed in terms of accumulated groundwater travel time
Pe is the Peclet number
D_e is the effective matrix diffusivity of radionuclide i
x is the penetration depth into the rock matrix
x_0 is the maximum penetration depth in the matrix
R_i is the retardation factor for radionuclide i in the rock matrix ($R_i = \varepsilon + K_d \rho$)
ε is the matrix porosity
K_d is the distribution coefficient of radionuclide i
ρ is the bulk density of the rock (2700 kg/m^3 is assigned in the FARF31 code)
λ_i is the decay constant for radionuclide i.

The following initial and boundary conditions are applied:

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

when $\zeta -> \infty$ $c_i = 0$.

The inlet flow is given by:

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

The boundary conditions for the diffusional tubes are:

$$\left.\frac{\partial c_{p,i}}{\partial x}\right|_{x=x_0} = 0$$

$$c_{p,i}(x,\zeta,t)\Big|_{x=0} = c_i(\zeta,t).$$

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

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

FARF31 requires constant transport parameters along the entire stream tube. Thus when applying the code to a stream tube with a varying water flux, constant effective parameters must be determined by suitable averaging techniques. The averaging involves weighting both the surface area between the flowing water and the rock, the length of the one-dimensional diffusion tubes, the water flux and the Peclet number. Concerning the dispersive term an approximation is made assuming that the ratio dispersion length over water velocity may be averaged along the stream tube:

$$\frac{D_L(z)}{U_f(z)^2} \approx \frac{\overline{D_L(z)}}{U_f(z)^2} = \frac{1}{z_0}\int_0^{z_0}\frac{D_L(z)}{U_f(z)}\frac{dz}{U_f(z)} \approx \frac{z_0}{z_0^2}\frac{\overline{D_L(z)}}{U_f(z)}\int_0^{z_0}\frac{dz}{U_f(z)} = \frac{t_w}{Pe}.$$

The approximation could partly be justified by the assumption of a constant dispersion length along the stream tube.

3.2 Numerical methods

The approach chosen for numerically solving the system of partial differential equations with boundary and initial conditions given above is a semi-analytical method dependent on three major steps. The method is illustrated in Figure 3-1.

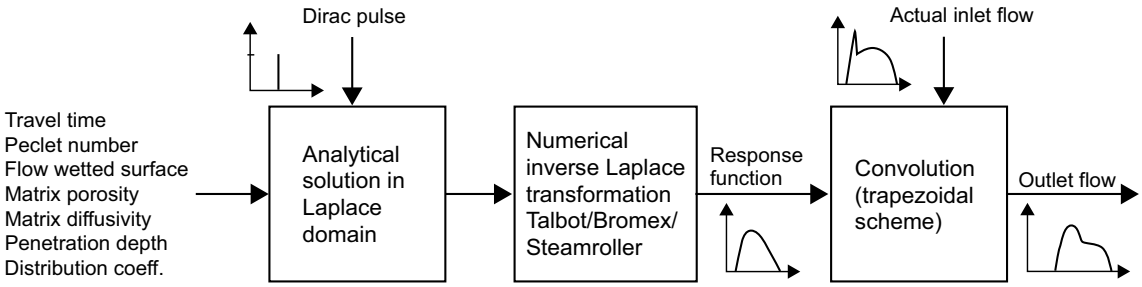

Figure 3-1. *Schematic illustration of the solution technique used in FARF31.*

In the first stage the analytical solution for a Dirac pulse input is calculated in the Laplace plane for the parent radionuclide as well as it contribution to the subsequent daughters. The analytical solution is numerically inverted to the real domain to obtain unit response functions. Three different algorithms for the Laplace inversion are available, the Talbot algorithm /Talbot, 1979/, the Bromwich inversion formula (BROMEX) /Gustafson, 1991/ and the Steamroller algorithm developed by /Dahlquist, 1993/. The unit response functions are then convoluted with the actual inlet flow to obtain the outlet flow of the parent radionuclide and any daughter it might have. If there is an inlet flow also of the daughters this is added to the amount produced from decay of the parents. The convolution of the two time series (response function and inlet flow) is performed with a straightforward numerical algorithm based on the trapezoidal rule.

4 Confidence in the model

The prime goal of model validation is to build confidence in the model concept and that the model is fit for its intended purpose. In other words:

- Does the model predict transport in fractured rock adequately to be used in repository performance assessments?
- Are the results reasonable for the type of modelling tasks the model is designed for?

Preferably, validation in this context is made by comparisons of model predictions with results from field experiments. For practical reasons, there are no experiments conducted in the time scale, which FARF31 is designed for, many thousands of years. In the available tracer experiments the time scale is short and thus effects such as rapid sorption, the detailed characteristics of the fracture and the flow field may dominate the results. Thus, the confidence building has to be based on other issues as well. Validation of FARF31 must therefore to a large extent be based on confidence in the manner in which its various component processes have been chosen, described and coupled together. In this section, model verification, comparisons with analytical solutions, and comparisons with other model concepts are also included.

4.1 Validity issues

Geometrical description

Transport of radionuclides in fissured rock occurs in complex network of fractures with widely varying physical, geological, geochemical and hydrological properties. In order to describe this in a mathematical model extensive simplifications are needed.

FARF31 is based on a stream tube dual-porosity approach, i.e. the radionuclide transport is assumed to take place along an imaginary one-dimensional flow path (stream tube). The stream tube encompasses both fractures with flowing water and the pore space within the rock matrix with presumed immobile water. The geometrical properties of the stream tube are given implicitly, e.g. the length is given indirectly by the groundwater travel time and the cross-section area is indirectly determined by the input flux. The modeller therefore has little control over the geometry of the stream tube, and in exceptional cases can the stream tube have a geometrical shape that infringes the basic assumptions. For example, in the case with an increasing velocity along the stream tube, the requirement of continuity in flow will cause the imagined tube to decrease in cross-section area. If the change along the stream tube is great, the basic assumption of no mixing between stream tubes is violated. As the effect of this is an overestimation of radionuclide release it may be acceptable. The opposite case with a decreasing water velocity is rather hypothetical and is not likely to occur under real conditions.

No detailed geometrical description of the fracture space within the stream tube is given. Instead, the effective area for interaction between the flowing water and the rock matrix is given as a parameter, the flow-wetted surface per volume of water. In the application of FARF31 within the SKB performance assessments, the water residence time is calculated assuming constant flow porosity within the entire rock domain. Thus, the water velocity is

proportional to the water flow rate (Darcy velocity) within the stream tube and the flow-wetted surface per volume of water is proportional to the flow-wetted surface per volume of rock. The basis for this assumption is that the later entity is believed to be more constant within the rock domain and is a more appropriate method for dealing with sorbing radionuclides. The drawback is that the groundwater travel time may be underestimated which may overestimate the release of non-sorbing radionuclides with short radioactive half-life.

Processes

The main processes included in FARF31 are advection, dispersion, matrix diffusion and sorption. Furthermore, radionuclide chain decay is included. These are the processes generally considered as most important for radionuclide transport in fissured rock. No new unknown processes that have an important influence on radionuclide transport are expected. The uncertainty is therefore largely connected to how the transport processes are modelled and which data are used for the model parameters. In Section 4.3 the use of the selected transport processes for SR 97 is further discussed.

Advection is a fairly straightforward process; solutes are carried by the flowing water. The conceptual difficulties appear when dealing with variation of advective velocities in space (or in time). In FARF31 advection accounts for the mean velocity, while any variations are attributed to dispersion as generally done in the advection-dispersion model. Since variations in flow occur on all scales, this division depends on the scale considered for the stream tube.

The applicability of the advection-dispersion model on which FARF31 is based has been debated, see for example /Neretnieks, 2002/. The main issues being that the Fickian-type of dispersion obtained using the advection-dispersion model gives some effects that contradicts observations or gives unphysical behaviour. The dispersion given by a dispersion coefficient, dispersion length or Peclet number is a lumped process taking into account spreading of a pulse due to velocity differences between different flow paths and within flow paths. Usually molecular diffusion is also included although it is normally of minor importance. One of the concerns with the advection-dispersion model is that it does not predict the increase of the dispersion length with distance that is observed in tracer tests. Thus, extrapolation to longer travel distances can underpredict dispersion if appropriate modification of the dispersion coefficient is not made. In FARF31 dispersion is defined by the Peclet number and thus the dispersion length is indirectly adjusted for the travel distance. Furthermore, alternative model concepts that can predict an increasing dispersion length with travel distance has been found to give very similar results for non-sorbing radionuclides using equivalent Peclet numbers. Another concern with the advection-dispersion model is that it predicts an upstream dispersion of solutes, which for cases with large dispersion can lead to unphysical results.

The modelling of matrix diffusion is based on the physical laws of diffusion. Sorption is modelled as linear equilibrium sorption. The main simplifications being that the matrix is assumed to be one-dimensional, have constant properties with depth and have properties that can be averaged along the entire flow path and are constant in time. In reality there will be a multitude of geological materials in contact with the flowing water with different effective dimensions, diffusion and sorption properties, also including zones with stagnant water. Different materials will be effective at different time scales and will also be different for different radionuclides depending on their sorptive properties. In principal, the choice of parameter values should be based on an evaluation of the effective matrices for the problem studied. In practice, values for undisturbed rock have been used, as it is believed to have the largest capacity for sorption but with a low transfer rate. Thus, conservative estimates of the breakthrough time will be obtained.

Surface sorption is not included in FARF31. Surface sorption considers geological materials on which sorption is so fast they can be considered to be in concentration equilibrium with the flowing water. Neglecting surface sorption is a conservative assumption.

Radioactive chain decay is a physical process that is in practice independent of the transport and retardation processes. However, since radioactive decay changes the chemical element and thereby the sorption properties, it needs to be solved in a coupled manner.

Model parameters

The properties of the rock and fractures within the stream tube are averaged over its entire length, by applying a flow-weighted averaging. The basis for this concept is that effective averaging of parameters can be performed and that suitable values can be derived. This is an important validation issue since a number of important parameters are difficult to measure directly and others can only be measured in points or in laboratory samples.

It can be shown that matrix interaction properties along a flow path can be integrated to an effective value. This is often expressed as the integrated ratio between the flow wetted surface and the water flow (also called the F-ratio or Beta-value). For cases where the matrix depth can be considered as infinite also diffusion and sorption parameters may be integrated along the flow path to obtain an effective value. This means that it is possible to derive effective parameters for sorbing radionuclides incorporating the total matrix effects along a flow path. This approximation is strictly valid only for cases with no dispersion, but gives a good approximation as long as dispersion does not dominate the transport. Calculations have shown that the approximation is acceptable at least for Peclet numbers as low as 2 /Elert et al, 1998/. Although the F-ratio is not directly used as input in FARF31 a similar effect can be obtained by setting the residence time and the flow-wetted surface so that their product corresponds to the F-ratio.

In the stream tube concept the average flow along the stream tube is considered. In practice, the flow within the stream tube may be divided into several flow paths. The F-ratio (ratio between the flow wetted surface and flow rate) may differ substantially between these flow paths, which may give very different impact on retardation of sorbing radionuclides. Furthermore, the combined effect of all the flow paths may be very different from the results obtained using average values of flow wetted area and flow rate. This effect becomes more pronounced for strongly sorbing radionuclides /Neretnieks, 2002/.

Comparison with experiments

Transport models similar to FARF31 and more complex models have been used to predict and analyse different tracer tests. In Sweden, tests have been carried out e.g. in the Stripa mine, at Finnsjön and at the Äspö HRL. Similar analyses have been performed internationally, e.g. within the framework of the INTRAVAL project /NEA/SKI, 1996/. However, transport processes that are of great importance for the results of the tracer experiments, such as the detailed geological structure of fractures or flow patterns, are of less importance for transport of long-duration releases of radionuclides, whereas the tracer tests commonly are less affected by matrix diffusion combined with sorption. The interaction mechanisms are, however, of great importance for large-scale release under natural conditions, even for non-sorbing solutes that have the ability to diffuse into the rock matrix. Hence, the comparisons cannot be used as direct evidence for the suitability of the models for safety assessment.

Evaluation of tracer experiments is difficult since many of the processes (matrix diffusion and sorption, diffusion into stagnant zones, hydrodynamic dispersion, sorption kinetics) have very similar effects on the breakthrough curves obtained from tracer experiments and cannot be discriminated in a single breakthrough curve. Experiments involving several tracers with different sorption properties, like those performed at the Äspö HRL, can to some degree be used to separate between some of the processes. However, a definite distinction between processes cannot be made due to experimental uncertainty, limited resolution in the tail end of the breakthrough curve, etc. Therefore, the understanding of radionuclide transport in a fissure has to rely on a combination of information from many types of sources, field observations, laboratory experiments, theoretical studies, etc.

4.2 Model verification

Results from FARF31 have been compared to analytical solutions and results from other numerical models. The analytical solutions are based on the advection-dispersion equation and the analytical model of /Tang et al, 1981/. The numerical model that was used to verify FARF31 is the multi-purpose model TRUMP /Edwards, 1972/. The evaluation has primarily been made by comparing the unit response function calculated by FARF31 with corresponding results from the alternative models. This provides a more sensitive method to compare model predictions than using results with other types of input functions. However, comparisons with other types of input functions have also been made in order to verify this part of the calculation chain.

4.2.1 Verification of FARF31 using an analytical solution

Comparison of unit response functions

In /Elert et al, 2001/ a large number of calculations are presented for which the relevant transport parameters are varied over a wide range covering the domain that is expected to be relevant for safety assessments. The unit response functions obtained from FARF31 were checked for consistency and mass balance. In general, the model behaved well, but some problems were identified and corrected. For a selection of cases the unit response function obtained with FARF31 were compared with analytical solutions. Here four cases are presented, Cases A to D. Two types of analytical models have been used for the model comparison:

- The analytical solution of the advection-dispersion equation with a retardation factor calculated assuming equilibrium sorption in the rock matrix.
- The analytical solution of the advection-dispersion equation including diffusion into an infinite matrix. Here, the analytical solution of /Tang et al, 1981/ has been used for comparisons. The solution can be classified as semi-analytical since a numerical integration is necessary.

The first type of model can be used to compare with FARF31 cases where a complete saturation of the rock matrix can be expected. These are cases with long travel time, high diffusivity and small maximum matrix penetration depth. Comparisons with this type of model are shown in Figure 4-1 to Figure 4-3.

The second kind of model /Tang et al, 1981/ can be used to compare with FARF31 cases when the penetration into the matrix is considerably less than the maximum penetration depth. Comparisons are illustrated in Figure 4-4 and Figure 4-5 for this type of situation.

Case A is based on a travel time of 100 years, a high dispersion (Pe = 2), small flow-wetted surface (a_w = 100 m^{-1}), a small penetration depth (x_f = 0.02 m) and a high matrix diffusivity ($D_e = 3.2 \cdot 10^{-5}$ m^2/s). In Figure 4-1 the unit response curve derived from FARF31 is compared with the analytical solution of the advection-dispersion equation with equilibrium sorption. The curves are identical except for the initial part when $K_d > 0$. In this case the assumption of equilibrium sorption is not valid, and the FARF31 curves show an earlier breakthrough as expected.

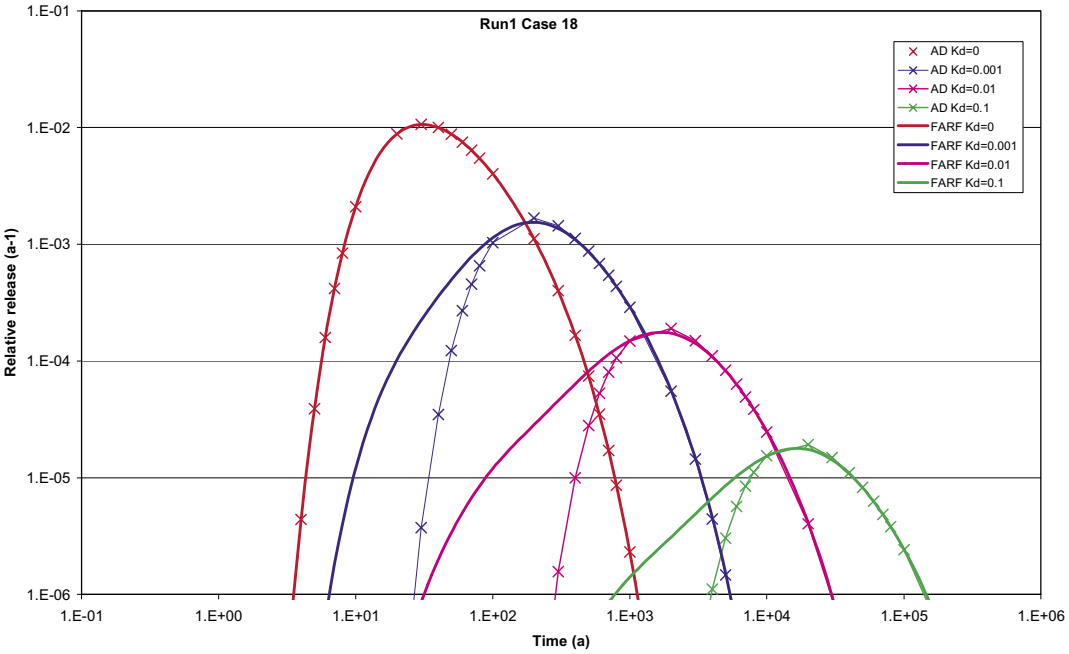

Figure 4-1. *Comparison of an analytical solution of the advection dispersion equation with equilibrium sorption and results from FARF31. Case A.*

Case B is identical to Case A except that the flow-wetted surface is larger (a_w = 10,000 m^{-1}). In this case the FARF31 unit response curves are identical to those of the analytical solution assuming equilibrium sorption, see Figure 4-2.

Figure 4-3 shows a comparison of FARF31 and the analytical solution assuming equilibrium sorption (Case C). The case is based on a travel time of 1000 years, a low dispersion (Pe = 40), large flow-wetted surface (a_w = 40,000 m^{-1}), a small penetration depth (x_f = 0.02 m) and a low matrix diffusivity ($D_e = 3.2 \cdot 10^{-8}$ m^2/s). The peak release of the two solutions coincides very well, but the FARF31 release occurs slightly earlier. FARF31 also have some numerical problems at the beginning and the end of the unit response curve, giving rise to oscillations in the tails of the unit response curve. The oscillation was examined in /Elert et al, 2001/. The oscillations seems to be connected to cases with very long travel times where a saturation of the matrix is obtained, i.e. short penetration depth and/or very high matrix diffusivity. The magnitude of the extra peaks are at least three orders of magnitude lower than the maximum release and should have little influence on the calculated release rates. However, the integral of the unit response function for some of the cases exceeds the expected value by about 10%.

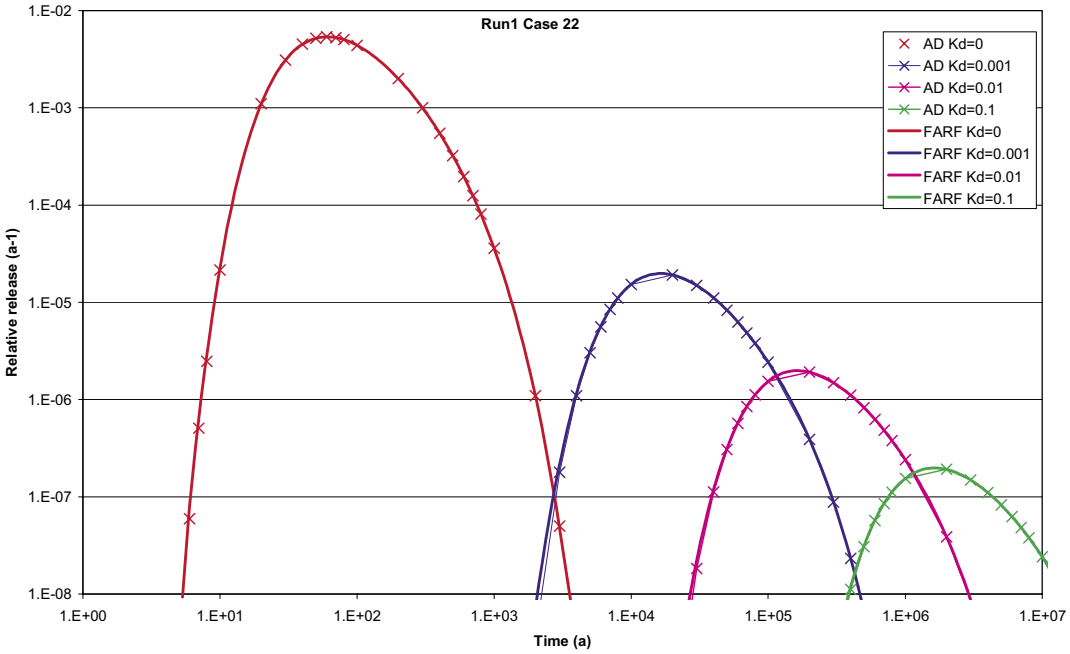

Figure 4-2. *Comparison of an analytical solution of the advection dispersion equation with equilibrium sorption and results from FARF31. Case B.*

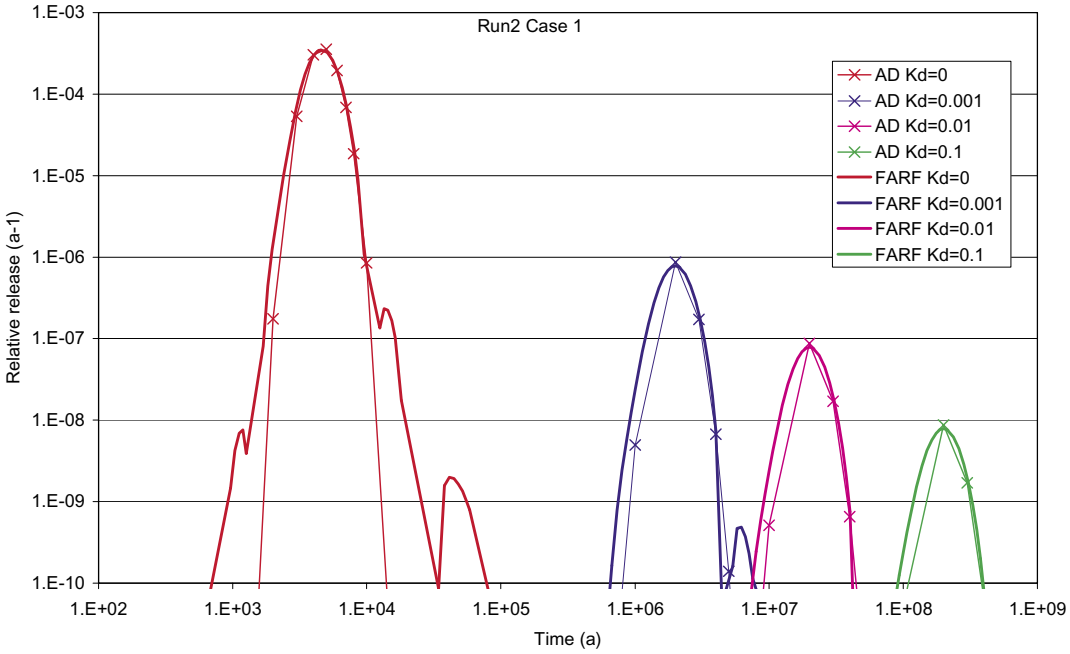

Figure 4-3. *Comparison of an analytical solution of the advection dispersion equation with equilibrium sorption and results from FARF31. Case C.*

In Figure 4-4 a comparison is made of the solution of FARF31 and the Tang solution including matrix diffusion for Case D. The case is based on a travel time of 100 years, a high dispersion (Pe = 2), small flow-wetted surface (a_w= 100 m^{-1}), a large penetration depth (x_f = 20 m) and a low matrix diffusivity ($D_e = 3.2 \cdot 10^{-8}$ m^2/s). The unit response curves calculated using the two methods give identical results.

A comparison has been made with an analytical solution describing a similar problem assuming an infinite matrix penetration depth /Tang et al, 1981/. In Figure 4-5 the analytical results are compared with FARF31 calculations with Pe = 10 and a maximum penetration depth of 2 meters. The solutions of the two models are nearly identical.

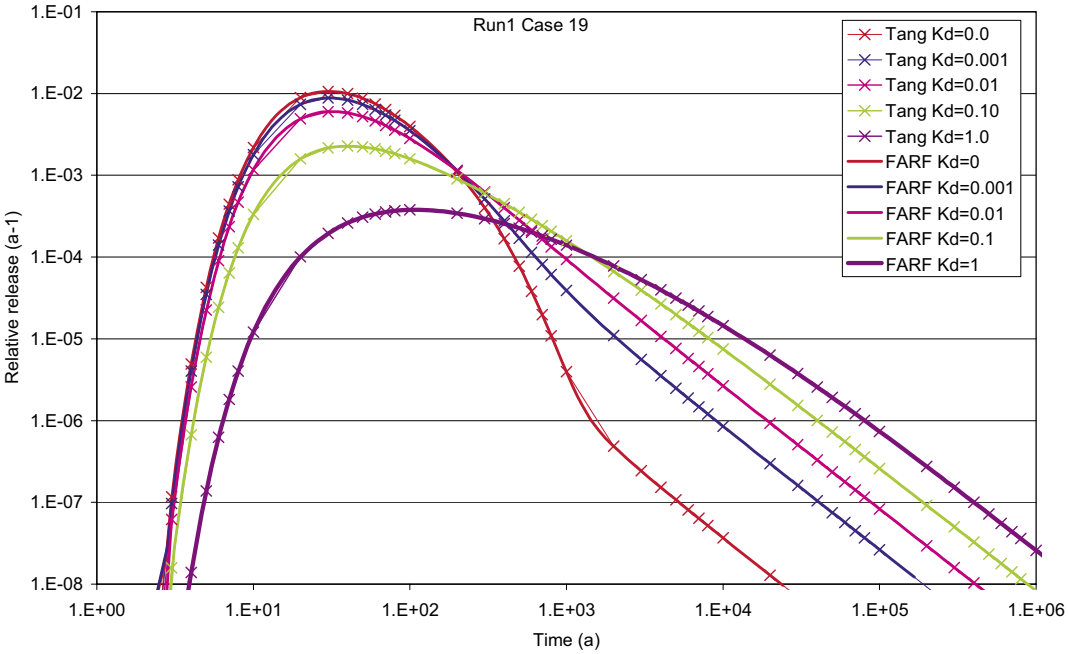

Figure 4-4. *Comparison of Tang solution of the advection dispersion equation with matrix diffusion and sorption and results from FARF31. Case D.*

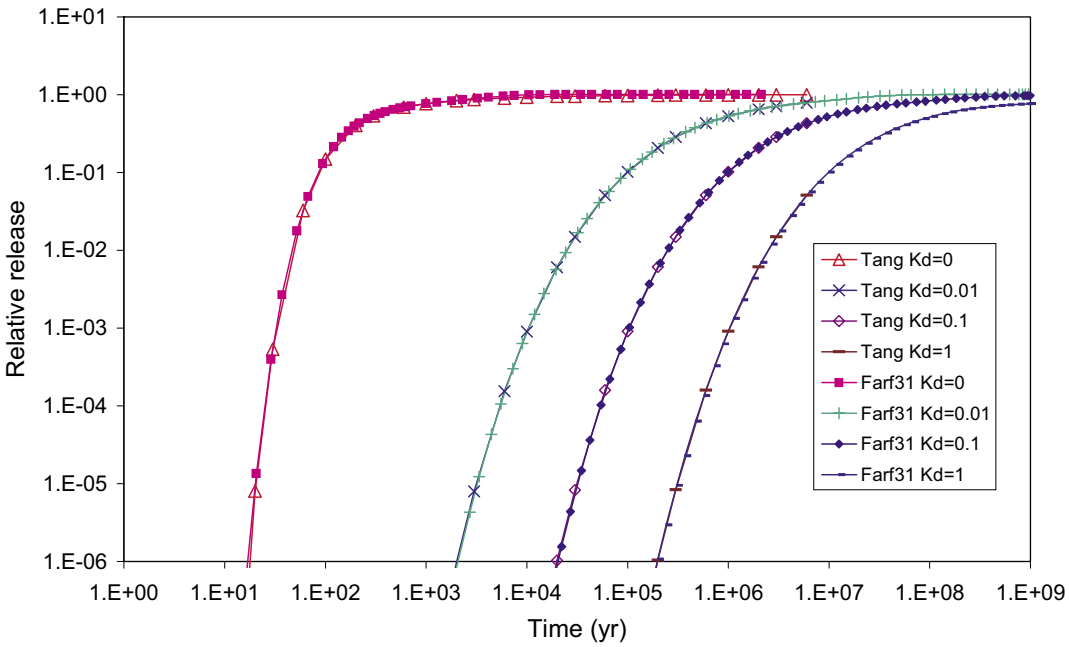

Figure 4-5. *Comparison of release curves from an analytical solution /Tang et al, 1981/ and from FARF31.*

Comparison of release rates

In /Eriksson et al, 1999/ the release rates of the nuclides in chain 4N+2 were calculated with FARF31 and compared to the analytical model /Tang et al, 1981/ where the chain decay was solved afterwards using an analytical solution of the Bateman equations. The input data were a travel time of 100 years, a Peclet number of 10, a flow-wetted surface of 1000 m^2/m^3, a porosity of 0.005, an effective diffusivity of $3.2 \cdot 10^{-6}$ m^2/yr for all nuclides, a penetration depth of 2 m and a K_d-value of 1 m^3/kg for all nuclides. The source term was initially 1 mole/year for each nuclide and then decreasing corresponding to the decay. The decaying source term was generated by numerically solving the Bateman equations. The analytical model /Tang et al, 1981/ can be used to compare with FARF31 cases when the penetration into the matrix is considerably less than the maximum penetration depth which is fulfilled in this case.

The release rates for all nuclides are shown in Figure 4-6. The difference between the solutions from FARF31 and Tang are small (most likely caused by the use of tabulated data as input) and hence these calculations can be seen as a verification of chain calculations with FARF31.

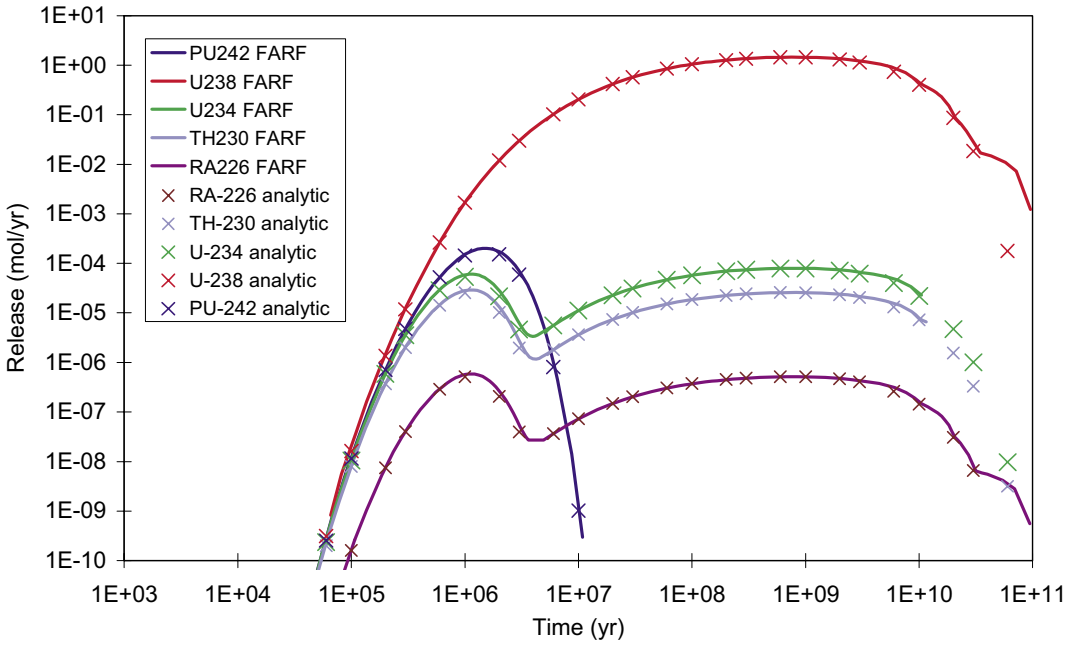

Figure 4-6. *Comparison of release rates for chain 4N+2 calculated with an analytical method and FARF31.*

4.2.2 Comparison with a numerical model

In /Elert et al, 1998/ a comparison was made of calculated unit response functions from FARF31 and the numerical code TRUMP /Edwards, 1972/: TRUMP is based on an integrated finite difference formulation. TRUMP calculates steady-state or transient mass or heat flow in one-, two-, or three-dimensions. In the present application TRUMP was set up to calculate solute transport by advection-dispersion with matrix diffusion and sorption. A comparison of the relative release rates obtained with FARF31 and TRUMP is shown in Figure 4-7. As may be seen the two curves follow each other well, with the exception of a slight deviation just before and at the release maximum.

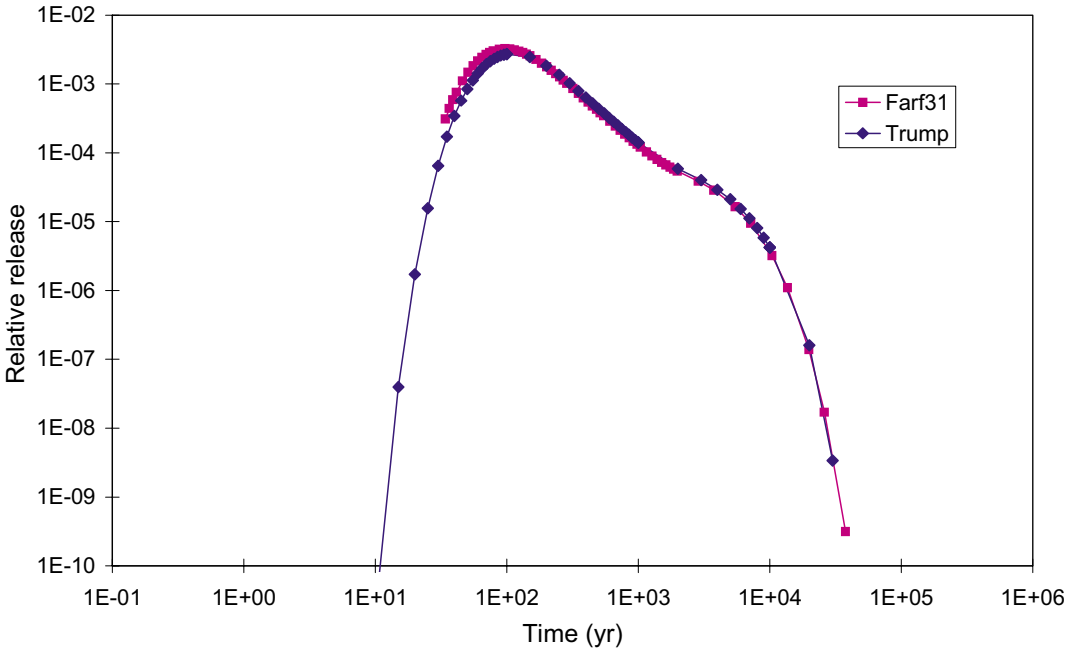

Figure 4-7. *Comparison of the response function from FARF31 and the numerical model TRUMP.*

4.3 Applicability to present use

Commonly, in performance assessments a large number of realisations of flow and transport is made to cover the associated uncertainties. Thus, the flow and transport including radioactive chain decay are preferably calculated in the same model framework. To be able to model the flow and radionuclide transport in the near field and far field of a deep repository, also including radioactive chain decay, a rather sophisticated concept is necessary if the relevant processes and mechanisms are to be considered. In order to avoid excessively long computational times there is a need for well-based simplifications.

In the SR 97 study, the model package PROPER was used for performance assessments of three hypothetical sites. PROPER includes a chain of models and is designed to handle multiple realisations and multiple canister locations in each realisation. For this reason, the far field code FARF31 is made relatively simple, and calculates the transport by using averaged entities to represent the most important processes. The lack of detail is partly covered by using a wide range of input data. The benefit is a relatively robust and fast far-field transport code.

A number of simplifications are included in the model FARF31. The model calculates radionuclide transport along an imagined one-dimensional flow path (stream tube) with constant flow. In the stream tube concept no mixing between stream tubes is considered, while the use of average values implies a full mixing between the flow paths within the stream tube. The use of the one-dimensional stream tube concept can be motivated by the small scale source term generally used in the SKB performance assessments. Radionuclide release is assumed to occur from individual canister positions in an underground repository. Furthermore, the locations of the failing canisters have been assumed to be randomly spread. The small source term can be expected to give rise to transport path lines of limited dimensionality motivating the use of a one-dimensional stream tube. The random location of the failing canisters to great extent reduces the motivation for a detailed description of the flow paths, as the actual details of the active flow path cannot be determined.

FARF31 uses groundwater travel time and near-field release as input data. For the considered flow path, the dispersion (represented by the Peclet number), the flow-wetted surface area (a_w), the matrix diffusivity (D_e) and the matrix porosity (ε) are given as effective flow-weighted averages, constant over the entire transport path.

It is concluded in /SKB, 1999/ that FARF31 handles all the relevant processes necessary for performance assessments that have been identified in the process description. The uncertainty is therefore mainly associated with how the transport processes are described and what data are used. In the safety study SR 97 it was stated that:

- The low colloid concentrations measured in granitic groundwater justify neglecting colloid transport.
- Sorption is a collective term for several processes for which the conceptual understanding varies. There is a large amount of laboratory data on sorption in the form of equilibrium sorption constants (K_d-values), but the process is more difficult to measure in the field. The approach in the performance assessment is to choose pessimistic K_d values so that the sorption capacity is not over-estimated.
- Uncertainties related to matrix diffusion and the porosity of the rock matrix is again handled by choosing pessimistic values. Many laboratory measurements of matrix diffusion and matrix porosity are available, but data from the field is more difficult to obtain.
- The geometric shape of the flow paths in the host rock is difficult to investigate and can only be described in a general sense. Thereby, the modelling of the flow paths is associated with uncertainty. This has a great influence on the important entity – the flow wetted surface. The uncertainty in flow was handled by setting up variants of the base case, where several stochastic realisations are performed in the created geometrical models. The uncertainty in the flow wetted surface was handled by pessimistic choices of data.

4.4 Alternative model concepts

4.4.1 Multidimensional models

An alternative to the stream tube approach is to use a two or three-dimensional transport code coupled to a groundwater flow model, either as two separate models or as an integrated model.

An advantage with a multidimensional transport model compared to the stream tube approach is that transversal dispersion between different stream tubes will be described explicitly. Multidimensional models are also more adequate for describing the release from extended sources. However, if the transport model is based on the advection-dispersion model many of the conceptual difficulties encountered with the stream tube approach remain, e.g. dispersion due to heterogeneity and variations in the actual flow paths in the rock is modelled implicitly by a dispersion term. The value of the dispersivity tensor has to be derived from other sources. The inclusion of matrix diffusion is not completely straightforward in a three-dimensional continuum model, since it requires an additional “dimension”. This is usually made by an independent set of nodes or elements perpendicular to the three dimensional net, which considerably increases the number of nodes or elements needed. Alternatively, matrix diffusion is described by an approximate solution. In both cases the contact area between the flowing water and the rock (flow-wetted

surface) must be described by an effective parameter representative for the averaging volume. A disadvantage with “full dimensionality” is the large computational effort needed to solve the three dimensional transport equations. The problem is time-dependent and generally the numerical solution of the transport equation requires finer discretisation than what is needed for the groundwater flow.

A number of two- and three-dimensional models have been developed that can handle stationary and instationary groundwater flow coupled with transport described by the advection-dispersion equation, e.g. NAMMU /Cliffe et al, 1998/. The model has the capability to model saturated and unsaturated groundwater flow in three dimensions. Transient contaminant transport may be modelled, including the effects of advection, diffusion, longitudinal and transverse dispersion, sorption and radioactive decay. In addition, fully coupled saline calculations are possible, for example for modelling the upflow of deep salt water during repository operation, so called upconing. NAMMU handles decay chains, and allows solubility limitations, which makes it possible to include interacting decay chains. STAFF3D is a 3-D finite-element model that simulates groundwater flow and the transport of conservative/reactive solutes in fractured or granular porous media. The contaminant transport module may account for advection, hydrodynamic dispersion, linear equilibrium sorption, and first-order degradation. Transport of a single species or members of a decay chain can be handled /Huyakorn et al, 1983/.

Alternatives to the advection-dispersion model exist, e.g. the multi-rate models /Haggerty and Gorelick, 1995; Haggerty and Reeves, 1998/ and particle tracking models /Svensson, 2001/. These modelling approaches have the potential to significantly reduce the computational effort.

Stochastic continuum groundwater flow models coupled to a two- or three-dimensional transport model account for macroscopic dispersion caused by spatial heterogeneity in the hydraulic conductivity. However, small scale dispersion is often included in the transport model. These models predict dispersion that is non-Fickian in nature. The advantage compared to the stream tube approach is that macroscopic dispersion and mixing of flow path are explicitly modelled. However, the stochastic continuum model does normally only give a large scale picture of the water flow in the rock, i.e. in the order of the block size used. Thus, dispersion due to variations in flow between individual flow paths must be modelled implicitly by the dispersion term in the transport equation. The problems with incorporating matrix diffusion as described above also apply for this type of model.

4.4.2 Discrete models

Discrete fracture models have been developed to obtain a better understanding of the water flow and radionuclide transport at a more detailed level. The idea is to describe the individual flow paths as physically correct as possible. Large-scale properties of the rock, such as dispersion, are thus a result of the properties assigned to the individual flow paths. A main reason for this modelling approach is to obtain a more realistic description of the scale behaviour of the radionuclide transport. Scaling of results from tracer experiments to repository conditions is an important step in the far field modelling.

Channel network model

The simplest discrete model is the channelling model, which is based on the idea that the water flows in quite widely separated channels, which may extend for considerable distance without intersecting other channels. The channels are assumed to be one-dimensional and no mixing is assumed to occur between channels before they reach the point of release. The

transport in each channel is calculated individually and the total release rate is obtained by adding the release rate from all channels. Alternatively, the channels are grouped according to flow rate and the release from each group is calculated and multiplied by the fraction of water flow in the group.

The channelling model predicts a scale dependent dispersion coefficient, proportional to the distance. This corresponds to using a constant Peclet value along the transport path in the advection-dispersion model. The dispersion behaviour of the two models may differ if surface sorption is considered. In the channelling model it is often assumed that the surface area available for surface sorption is inversely proportional to the channel aperture. Thus, the largest channels with high flow rates and short water residence time will have low retardation factors, while smaller channels with low rates and long residence times will have high retardation factors. This will lead to an increased spreading of the breakthrough curve. The effective dispersion may thus be different for radionuclides with different sorption properties.

Discrete network models

A network of fractures or channels is generated stochastically in a three-dimensional space. The fractures are often modelled by simple geometrical structures such as discs or rectangles. The models need data such as frequency, orientation, dimension and transmissivity. Channelling may be described by modelling discrete flow paths within the fracture planes. The transport within the individual network segment is usually described by the advection-dispersion model. However, the dispersion within an individual flow path is often considered to be of minor importance compared to the dispersion caused by variations between channels, and is therefore treated in a simplified way or even neglected. The effect of surface sorption can easily be included into fracture network models, but the inclusion of matrix diffusion is more complex, especially in large networks.

A discrete network model may be able to calculate the transport and rock interaction for each section of the model geometry, which means that the total transport time is the sum of the individual sections. In addition dispersion can directly be simulated and not described by a model parameter. The code CHAN3D /Gylling, 1997/ handles flow and transport in a network of channels. Dispersion is simulated by differences in conductivity between the flow paths, by mixing at channel intersections and by the interaction mechanisms. For each channel the rock interaction is calculated as matrix diffusion and sorption. Decay of single nuclides is implemented and input from a near-field concept e.g. COMP23 can be used. The discrete concept NAPSAC /Hartley et al, 2002/ calculates flow and transport in network of fractures. Radioactive decay is not implemented yet. As FRACMAN /Dershowitz et al, 1985/ it can estimate the flow-wetted surface for each traversed fracture which enables rock interaction calculations. Transient conditions and rock interactions are included. FRACMAN's module for performance assessments can handle radioactive decay.

5 Documentation and code administration

FARF31 can be used as a component in the model chain PROPER or stand-alone. As for other models in the PROPER package documentation, a source code control system, and test cases are available. The documentation describes handling and updates of the code. Test cases are constructed which can be used to check updates and be used as templates. The development of the code is kept under source code control.

5.1 Documentation and publications

The basis for the first version of FARF31 is given in /Norman and Kjellbert, 1990/. In /Elert et al, 1998/ possibilities for developments were investigated, e.g. division of stream tubes into sequential segments which may be defined in such a way that they have more homogeneous properties. Another option was to find better methods to derive effective transport parameters for the stream tubes.

FARF31 has been updated to handle nuclide specific effective diffusivities /Eriksson et al, 1999/. In another project, work was made to improve and test the code further /Elert et al, 2001/. Recently, the User's Guide /Lindgren et al, 2002/ to FARF31 has been updated to include the improvements. The User's Guide is also available on-line.

5.2 Source code control

The development of FARF31 is under strict control using the Unix Source Code Control System (SCCS). This means that it is possible to keep track of every modification and to come back to an earlier version if that is needed. Based on SCCS there is a build environment available for the developer. The build environment enables that the developer works with a copy of the newest code version. A new development can then be checked by running the available test cases. If the new development passes the test examples, the main source code is updated and the modification is documented.

5.3 Development using test cases

A number of test cases have been set up for FARF31 in the test batch. The test batch is described in the User's Guide /Lindgren et al, 2002/. The tests cover both simplified cases and complete performance assessment cases. One of the test cases is a batch of cases which is intended to test the code performance within a wide range of parameter values. Six input parameters are varied; water residence time, Peclet number, flow-wetted surface, effective diffusivity, matrix penetration depth and distribution coefficient.

An important objective of the test batch is to provide tests to be run after a code modification and hence verify that the new version is giving the expected results. After a code modification is made, the test batch should be executed to check that results are the same as prior to the modification of the code. By running the test batch several different features of the code are tested. The test batch contains cases that can be compared with analytical solutions and cases from performed performance assessments.

6 Discussion and conclusions

For FARF31, the ambition of the prevailing validation document is to use the same definition of validation as for other codes used for performance assessments of repositories. In general terms, validation can be described as the process of building confidence in the fitness of purpose of models that are used in performance assessment and hence in the results obtained from the models. The aim of validation in the context of performance assessment should be to demonstrate that the model is adequate for the purpose for which it is intended. Preferably, validation in this context is made by comparisons of model predictions with results from field experiments. Since there are not many experiments conducted in the field using radioactive solutes, the confidence building has to be based on other issues as well. In this report, model verification, comparisons with analytical solutions, and comparisons with other model concepts are also included.

FARF31 has been shown to be suitable for the performance assessments within the SKB studies. Among the advantages are that it is a fast, simple and robust code, which enables handling of many realisation with wide spread in parameters in combination with chain decay of radionuclides. As a component in the model chain PROPER it is easy to assign statistical distributions to the input parameters. Due to the formulation of the advection-dispersion equation in FARF31 it is possible to perform the groundwater flow calculations separately. A bootstrap function transfers the groundwater travel times calculated by the groundwater flow model.

In FARF31 the properties of the rock and fractures within the stream tube are averaged over its entire length, by applying a flow-weighted averaging. Thus, it is an important validation issue that effective averaging of parameters can be performed and that suitable values can be derived. It can be shown that matrix interaction properties along a flow path can be integrated to an effective value. For cases where the matrix depth can be considered as infinite also diffusion and sorption parameters may be integrated along the flow path to obtain an effective value. This means that it is possible to derive effective parameters for sorbing radionuclides incorporating the total matrix effects along a flow path. This approximation is strictly valid only for cases with no dispersion, but gives a good approximation as long as dispersion does not dominate the transport.

For some applications, such as simulations of field experiments, FARF31 may be too simplified. The concept of using stream tubes does not allow multiple paths arising from the heterogeneous rock from a single starting position. Furthermore mixing of fluids between paths is neglected in FARF31. Also the averaging of entities over the whole transport length may cause different results compared to using a more sophisticated concept that can solve flow and transport in the same framework. This can to some degree be circumvented by calculating the transport and rock interaction for individual sections of the model geometry.

FARF31 has been tested and compared with analytical solutions and other models and was found to correspond well for a wide range of input parameters. The model is deemed to be well suited for performance assessments within the SKB framework.

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