

Radionuclide migration in strongly fissured zones – The sensitivity to some assumptions and parameters

Anders Rasmuson and Ivars Neretnieks

Dept of Chemical Engineering, Royal Inst of Technology Stockholm August 7,1985

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BOX 5864 S-102 48 STOCKHOLM TEL 08-665 28 00 TELEX 13108-SKB RADIONUCLIDE MIGRATION IN STRONGLY FISSURED ZONES - THE SENSITIVITY TO SOME ASSUMPTIONS AND PARAMETERS

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RADIONUCLIDE MIGRATION IN STRONGLY FISSURED ZONES - THE SENSITIVITY TO SOME ASSUMPTIONS AND PARAMETERS

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SUMMARY

Radionuclides escaping from a repository for high level nuclear waste in crystalline rock may eventually be carried by the flowing water in fissure zones. In such zones the rock is broken in blocks of varying sizes and shapes. Also, the water velocity may vary considerably in such zones. A previously developed model which lumps the different blocks into a single PSEUDOBODY is tested by comparing it with an exact analytical solution which can account for the diffusion into blocks of any size distribution. The approximate simplified model which is based on a numerical scheme, and thus is more versatile, gives errors which are small compared to the "normal" variation in observed block size distributions and other data.

A method for determining an "average" Peclet number (or dispersion length) in a strongly varying velocity field is tested and found to give small errors compared to the present confidence limits in predicting dispersion data for large migration distances.

A simple criterion is proposed for defining the cutoff limit in the block size distribution, below which the blocks can be modelled as if they were in equilibrium with the flowing water.

A simple sensitivity analysis shows that much can be gained if the confidence limits for block size distribution, water flow rate, dispersion data, sorption data, and matrix diffusion data can be narrowed down.

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BACKGROUND

The Swedish concept for a repository for spent nuclear fuel is to emplace the fuel in copper canisters and to store these at large depth, typically 500 m, in crystalline rock. The bedrock is fissured even at these depths and water seeps through the fissures. At a larger scale - on the order of one kilometer apart - long zones have been observed, where the rock is more fissured than in the rest of the rock. These zones may be very long and extend to large depths. They are usually vertical or near vertical. These zones are called lineaments.

The repository will be situated in less fissured rock. If the copper canisters degrade and water contacts the spent fuel, the radionuclides may be leached by the seeping groundwater. The radionuclides will first move in the "good" rock and then eventually emerge into the lineament. The lineament is more porous, more fissured and there are also parts where the rock has been crushed into small particles. The surface area available for sorption in the lineament may be considerably larger per water volume than in the "good" rock. This may enhance sorption and nuclide retardation. On the other hand, there may be parts of the lineament where the water movement is upwards and as the seepage rate is larger, the residence time of the water may be shorter. This gives less time for nuclide interaction with the rock matrix.

In a previous paper (Neretnieks and Rasmuson, 1984) the impacts of strongly varying velocities and block sizes along the flow path were investigated. The Integrated Finite Difference Method (IFDM) was used in the calculations. This numerical scheme can, in principle, handle any velocity field and block size distribution "exactly". This would, however, require extensive computer time and memory space. An attempt was made to account for blocks of various sizes by the MINC (Multiple Interacting Continua) approach. This method accounts for the large sorption surface but small volume of small blocks and small surface area but large volume of large blocks.

The purpose of the present paper is to investigate some simplifying assumptions in greater detail. To this end a recently derived analytical solution (Rasmuson, 1985b), taking into account any block size distribution, is utilized.

THE PHYSICAL SITUATION AND MODELLING APPROACH

The physical situation is treated at length by Neretnieks and Rasmuson (1984). It is only outlined here. Crystalline bedrock has been observed to be fissured on several scales. There are the large scale lineaments at distances of kilometers apart or more with widths of up to several tens of meters. Their vertical extension can probably be many kilometers and the lineaments can often be followed for many kilometers or tens of kilometers on the ground surface. In the lineaments the rock is broken and crushed and consists of blocks of various sizes. There may be a considerable amount of "fine" material. This has been observed in all the areas investigated in Sweden for the Nuclear Fuel Safety project (KBS, 1983). The bodies of rock between the lineaments are also fractured, but the fractures are usually at larger spacings than within the lineaments and the rock is on the average less permeable (KBS, 1983).

The hydraulic conductivity of the lineaments as well as of the "good" rock decreases with depth. Also the driving force for the water movement - the hydraulic gradient - decreases with depth (Carlsson et al., 1983).

In principle, it is possible to do rigorous calculations of the three dimensional flow field and to superimpose the transport equations on the flowlines in a full three dimensional calculation, including the effects of velocity dependent dispersion tensor and the effects of interaction by the radionuclides with rock blocks of different sizes

along the flow path. In fact, rigorous three dimensional flow path calculations have been performed for such cases (Carlsson et al., 1983) and there are model formulations which account for the above effects for nuclide transport (Hopkirk and Gilby, 1983; Neretnieks and Rasmuson, 1984). There also seem to be no difficulties in principle to fully incorporate them into existing codes. The major drawbacks at present seem to be that larger computer memories and computing times are needed and that the results may not be quite as transparent as when only a few effects must be accounted for. In some cases not all effects may be of importance for predicting radionuclide transport and it may be advantageous to have simpler, more transparent models for scoping calculations and for studying the relative importance of the various variables. At present the data on the hydraulic conductivity, lineament widths and block size distribution, fissure spacing, channeling effects and several other quantities are not very accurately known. It may also be expected that for some of the quantities the natural variation in the data is considerable. For practical reasons many of the data will be obtained by sparse sampling. The standard deviation of, for example, the hydraulic conductivity has been found to be quite large (Carlsson et al., 1983).

In this study we attempt to investigate the impact of some simplifying assumptions which lead to considerably simpler computing schemes than the rigorous approach. We also attempt to compare the errors introduced by the simplifying assumptions with those due to natural variations in the data.

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MATHEMATICAL MODEL

The movement of the nuclide in the rock can formally be described by the following equation

$$\frac{\partial C}{\partial t} + \bar{\nabla} \cdot C\bar{v} = \bar{\nabla} \cdot D\bar{\nabla}C - \Sigma S_k$$
(1)

 S_k denotes reaction mechanism number k. This formulation does not distinguish between the solid and the fluid phase and can in principle be applied directly to a heterogeneous medium by accounting for the material properties, velocities and reactions in the various phases. For example, this is done in the TRUMP-method (Edwards, 1972). Usually, it is preferred to distinguish the processes in the flowing phase from those in the solid phases. The coupling is then done at the boundaries between the phases. In the case where there is no concentration gradient perpendicular to the flow direction, equation (1) simplifies to

$$R_{a} \frac{\partial C_{f}}{\partial t} + V \frac{\partial C_{f}}{\partial z} - D_{L} \frac{\partial^{2} C_{f}}{\partial z^{2}} = -R_{a} \lambda C_{f} - S$$
(2)

Equation (2) accounts for the interaction with the solid by instantaneous reversible surface sorption, advection, Fickian type dispersion, decay and some as yet not defined reaction S. Equation (2) is extended to apply to a nuclide in a chain in a straightforward manner by adding a term $R_a^* \ \lambda^* C_f^*$ on the right hand side which accounts for the production of the nuclide under consideration from its mother nuclide. S accounts for the depletion of the nuclide in the water due to the diffusion into the porous water-saturated rock.

$$S = -\frac{1}{m V_{s}} \int_{A'} D_{p} \varepsilon_{p} \frac{\partial C_{p}}{\partial \bar{n}} dA'$$
(3)

where $V_{\rm S}$ is total solid volume and A' interfacial surface in the control volume.

 \bar{n} is the inward directed normal at the surfaces of the solid in contact with the water in the control volume. The integration is made over all the surfaces within the control volume. The formulation of equation (3) is quite general. For regular bodies such as infinite slabs, cylinders and spheres, S becomes:

for a continuous distribution

$$S = -\frac{1}{m} \int_{0}^{\infty} \frac{\alpha_{f}^{+1}}{b} f(b) D_{p} \varepsilon_{p} \frac{\partial C(b)}{\partial x} \Big|_{x=0} db$$
(4a)

and for a discrete distribution

$$S = -\frac{1}{m} \sum_{i} \frac{\alpha_{f}^{i+1}}{b^{i}} F(b^{i}) D_{p}^{i} \varepsilon_{p}^{i} \frac{\partial C_{p}^{i}}{\partial x} |_{x=0}$$
(4b)

 $\alpha_{\rm f}$ is 0, 1 or 2 for slabs, cylinders or spheres respectively. For the individual size fraction "i" the transport equation (1) can be written

$$\kappa^{i} \frac{\partial C_{p}^{i}}{\partial t} = \frac{1}{r^{\alpha}_{f}} \frac{\partial}{\partial r} \left(r^{\alpha}_{f} D_{p}^{i} \varepsilon_{p}^{i} \frac{\partial C_{p}^{i}}{\partial r} \right) - \kappa^{i}_{\lambda} C_{p}^{i}$$
(5)

Equation (5) is written in this way for future reference. It is coupled to equation (2) by the relation

$$C_p^i = C_f$$
 at $r = b^i$ (6)

The surface and volume retardation coefficients are defined by

$$R_a = 1 + K_a a \tag{7}$$

$$K = \epsilon_{p} + K_{d} \rho_{p} (1 - \epsilon_{p})$$
(8)

To evaluate S in equation (4) it is in principle necessary to evaluate equation (5) the same number of times, N, as there are size fractions if conventional numeric methods are used to solve the equations.

Rasmuson (1985b) has solved equations (2), (4b), (5) and (6) by analytical methods for some simple initial and boundary conditions:

$$u_{f} = u_{f}[\delta, Pe, R, \Lambda, y, b^{i}/b, F(b^{i})]$$
 (9)

where δ , Pe, R, Λ and y are dimensionless parameters based on the smallest block size and b^i/b and $F(b^i)$ specify the block-size distribution.

Equation (9) is actually a special case of a more general solution including, for example, size variable diffusivities and sorption capacities.

The solution (equation (9)) will be used here to study the errors introduced by the simplifying assumptions proposed and described in depth by Neretnieks and Rasmuson (1984). The basic assumptions for lumping the various block sizes into one shape seem to have first been proposed by Pruess and Narasimhan (1982). They called it the MINC (Multiple Interacting Continua)-approach. In the following we denote this approach the PSEUDOBODY-approach. In this method the blocks in an element of space are divided into a number of shells and it is assumed that all the shells, regardless of blocksize and shape, at the same distance from the surface behave alike. This is of course an approximation because the shape of the blocks influences the transport in a shell at a given distance, and even for the same shape a shell at a given distance reacts differently if the area ratio of adjacent shells is different (Neretnieks and Rasmuson, 1984).

The PSEUDOBODY-assumption makes it possible to construct equally sized pseudoblocks having a given area A(x) for diffusion at a distance x from their surface. The pseudoblocks have the same A(x) and the same volume as the real block size distribution in the element. For these pseudoblocks the transport equation (5) can be written

$$\kappa \frac{\partial C_p}{\partial t} = \frac{1}{A(x)} \frac{\partial}{\partial x} \left(D_p \varepsilon_p A(x) \frac{\partial C_p}{\partial x} \right) - \kappa_\lambda C_p$$
(10)

A(x) can be interpreted as the crossectional area normal to the transport direction in a pseudoblock at a distance x from the block's surface. For real regular bodies like infinite slabs, cylinders and spheres $A(x) \alpha r^{\alpha f}$ if the distance from the surface is exchanged for the radius. Equation (10) can now be used once instead of using equation (5) N times to evaluate S.

It is interesting to note that even for a uniform blocksize distribution the PSEUDOBODY-approach is exact only for "smooth" block shapes such as spheres, infinite cylinders and slabs, but not for shapes with corners and edges such as cubes or square rods. For spheres, or cubes, with diameter 2b the cross-section for diffusion A(x) at distance x from the surface is given by:

$$A(b,x) = V_{s} \frac{3}{b} (1 - \frac{x}{b})^{2}; \qquad 0 \le x \le b$$
(11)

If we have a distribution of spherical blocks we obtain:

$$A(x) = \sum_{i}^{\infty} A(b^{i}, x) = \sum_{i}^{\infty} V_{s}^{i} \frac{3}{b^{i}} (1 - \frac{x}{b^{i}})^{2}$$
$$= V_{s} \sum_{i}^{\infty} F(b^{i}) \frac{3}{b^{i}} (1 - \frac{x}{b^{i}})^{2}; \quad 0 \le x \le b^{i}$$
(12)

Introducing these results into equations (2) and (10) we obtain for constant $D_{\rm D}\varepsilon_{\rm D}$

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$$R_{a} \frac{\partial C_{f}}{\partial t} + V \frac{\partial C_{f}}{\partial z} - D_{L} \frac{\partial^{2} C_{f}}{\partial z^{2}} = \frac{1}{m} \left\{ \Sigma \frac{3}{b^{i}} F(b^{i}) \right\} D_{p} \frac{\partial C_{p}}{\partial x} \Big|_{x=0}$$

$$- R_{a} \lambda C_{f}$$
(13)

and

$$K \frac{\partial C_{p}}{\partial t} = \frac{D_{p} \varepsilon_{p}}{\frac{3}{b^{i}} F(b^{i})(1 - \frac{x}{b^{i}})^{2}} \frac{\partial}{\partial x} \left\{ \Sigma \frac{3}{b^{i}} F(b^{i}) (1 - \frac{x}{b^{i}})^{2} \frac{\partial C_{p}}{\partial x} \right\}$$
$$- K \lambda C_{p}$$
(14)

for $0 \le x \le b^i$

We can here again see the gross simplification of the governing equations for cubes and spheres compared to the rigorous solution. For cubes the simplification is even larger than for spheres because the equation of diffusion in a cube requires more computing effort than for a sphere. In cases where not only the size of the blocks varies but also their shape, a PSEUDOBODY type approximation seems to be attractive. Unfortunately, the equations above do not seem to have reasonably simple analytical solutions. It can be seen in equation (12) that A(x) is readily evaluated if $F(b^{i})$ is known for the block size distribution. In practice A(x) may be fitted to some simple function, e.g. a polynomial or spline polynomial function, to further reduce the computing effort. If $D_p \varepsilon_p$ also varies with x, the product $D_p \varepsilon_p A(x)$ can be handled in the same way.

COMPARISON BETWEEN THE PSEUDOBODY APPROXIMATION AND THE EXACT SOLUTION

The two methods are compared by investigating the differences in the effluent concentration of Np-237 for some sample cases. The same data are used for these calculations as were used by Neretnieks and Rasmuson (1984). They are summarized in Table 1.

The physical situation modelled is the flow in a lineament which contains two blocksizes and is also in contact with the surfaces of the "good" rock on both sides of the lineament. Note that in the analytical solution, the blocks are approximated by spheres. The PSEUDOBODY approach does not distinguish between cubes and spheres.

Two block size distributions are used. In the one called "Small" the fines are made up of 0.02 m blocks. In "Large" the fines consist of 0.1 m blocks. In all other respects the two distributions are alike.

In this example the water velocity and dispersivity are assumed to be constant in order to utilize the analytical solution exactly. The influence of varying water velocity will be investigated separately below. The data are summarized in Table 2. The initial and boundary conditions used assume zero initial concentration of Np-237 and at times larger than zero the inlet condition is a decaying band release with infinite duration. $C(z=0) = C_0 \cdot e^{-\lambda t}$ for t> 0.

	Block size diameter m	Number of blocks in REV*	Volume fraction F(b ⁱ)	Outer surface area A(b ⁱ) in REV m ²
Case	0.02	9375	0.0909	22.5
"smal	ו" ל0.5	6	0.9091	9
	(∞ (200)**	(2)	-	0.5
Case	(0.1	75	0.0909	4.5
"large	e" 70.5	6	0.9091	9
	L∞ (200 m)*	** (2)	-	0.5

- * The representative elementary volume (REV) is 3.3 m wide, 0.5 m high and 0.5 m long. It also includes two surfaces from which diffusional transport takes place into two very large blocks.
- ** In the exact solution the very large blocks are modelled by a part of a large sphere (diam = 200 m). Since the penetration depth is very small in comparison to the radius the flat walls adjacent to the lineament are accurately accounted for. The volume of these blocks is not included in the REV.

Table 1. Data used for comparison of exact solution and PSEUDOBODY approach.

Parameter	Dimension	Value
Travel distance, L	m	475
Water residence time, t _w	S	7.8125•10 ⁷
Peclet number, Pe	-	21.875 and 0.875
Surface retardation coefficient, R _a	-	1
Volume equilibrium coefficient, K	m ³ /m ³	1.35•104
$D_p \epsilon_p = D_e$ Half life of Np-237, T _{1/2} Flow porosity, ϵ_f	m ² /s years	5•10 ⁻¹⁴ 2.14•10 ⁶ 5•10 ⁻⁴

Table 2. Data used comparing exact and PSEUDOBODY solutions.

The results at z = L are depicted in Figures 1 and 2. The agreement is surprisingly good. The PSEUDOBODY approach tends to give somewhat earlier breakthrough in this case compared to the exact solution, but the peak is very accurately predicted. It may be noted that there is a noticable difference between the two cases "Large" and "Small" as there is an impact of the size of the fines in this case. Fines mainly influence the early part of the breakthrough curve.

Two conclusions are drawn from the results. The PSEUDOBODY approach should be a powerful tool in numerical calculations with block size

distributions, especially where chain decay must be accounted for, as compared to "exact" numerical calculations where every block size and shape must be accounted for separately. This will significantly reduce the computing effort. For single species the analytical solution should provide a powerful tool when very accurate calculations are needed.

DISPERSION IN A VARYING FLOW FIELD

The analytical solution used in the previous analysis is derived for the case of constant velocity. This solution is also exact for the case with no dispersion but variable velocity. Neretnieks and Rasmuson (1984) showed this by introducing

$$\zeta = \int_{0}^{z} \frac{dz}{V(z)}$$
(15)

to transform the velocity into a residence time. If the "dispersion" is caused mainly by channeling effects and the Fickian type of dispersion is small in comparison (Neretnieks, 1983) even very large "dispersion" effects may be modelled exactly by the transform (15) in a flow field with arbitrarily varying velocity.

When Fickian type dispersion cannot be neglected numerical methods must be used at present in cases where the velocity varies along the flow path. The longitudinal dispersion may be approximately accounted for in a varying flow field by using the following averaging method (Neretnieks and Rasmuson, 1984):

$$Pe = \frac{t_w^2}{\alpha \int_0^L \frac{dz}{\lfloor V(z) \rfloor^2}}$$
(16)

This average is based on the method of adding variances of flow sections coupled in series (Levenspiel, 1972). The idea has been carried to its extreme by making the flow sections infinitesimally small. This approximation improves as the dispersion coefficients decrease.

The effects of these approximations are also shown in Figures 1 and 2 for the cases defined in Tables 2 and 3. The dash-dot line shows the results of a "proper" numerical handling of the dispersion in a variable flow field. The dispersion length in this case is kept constant - 250 and 10 m respectively - along the flow path with varying velocity. In the approximate calculations using equation (16) and constant velocity (but the same residence time) the equivalent average dispersion lengths are 542.86 m and 21.71 m respectively. The results for these cases are given by the dashed lines in Figures 1 and 2. Considering that the averaging has been done over a velocity ratio span of 8000, the differences are surprisingly small.

Parameter	Dimension	Value
Dispersion lengths, α	m	10 and 250
Hydraulic gradient, i	m/m	1/Z for Z>25
Water flux, V _O	m ³ /m ² •s	0.1/Z ³ for Z>25
Water residence time, t _w	s	7.8125•10 ⁷

Table 3. Additional data for the varying velocity case.

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A CRITERION FOR TREATING THE DIFFUSION INTO SMALLER BLOCKS AS INSTANTANEOUS

It would be useful to have a criterion for deciding when the instationary saturation phase of the smaller blocks in the lineament must be accounted for. If the travel time is long in comparison to the equilibration time, the uptake of the smaller blocks may instead be modelled as instantaneous with a retardation factor R_a appearing in the transport equation. This would save computer time (and discretization work) especially in the case of chain decay where a numerical solver must be used. Due to the complicated situation such a criterion has not been derived exactly.

A first indication of what penetration distances to expect during a certain contact time can be obtained by solving equation (5) for the concentration profile in a semi-infinite slab particle which suddenly is contacted with a fluid having concentration C_0 of a stable tracer. The solution is (Bird et al. 1960, p. 354):

$$C/C_{0} = \operatorname{erfc}\left(\frac{x}{\sqrt{\frac{D}{K}} \epsilon_{p}}\right)$$
(17)

It is valid for cases when the penetration depth is small in comparison to the size of the body. Here, we use the approximation that the part of the body where the concentration would become larger than 0.48 C_0 , during a certain contact time Δt , can be said to be instantaneously equilibrated. The argument is 0.50 in equation (17) for this C/C₀. The "equilibrated" depth η_e is then directly obtained from equation (17):

$$\eta_{e} = \sqrt{\frac{D_{p}\varepsilon_{p}}{K}} \Delta t$$
(18)

The problem is then reduced to determining the contact time Δt to use in equation (18). If the release is constant in time and takes place during a known time interval, T_{leach} , then this can be used. For an infinite decaying band release the number of halflives, $T_{1/2}$, might be used after which the concentration has decayed to insignificant values. After 3 halflifes the activity is 1/8. Here it will be attempted to use $\Delta t = 3 T_{1/2}$. A comparison is made below between the exact solution and a solution where the blocks with a radius smaller than n_e are assumed to be at all times in equilibrium with the flowing water. This tests if the chosen Δt :s are reasonable.

Using the data in Table 2 we find $n_e = 0.027$ m for Np-237. This means that blocks twice this size would be instantaneously equilibrated. In the example with the small blocks (0.02 m) these might well have been included in the surface retardation factor R_a . In Figures 3 and 4 the analytical solution (Rasmuson, 1985b) with three blocksizes, is compared with the case where the smallest blocks in each distribution are taken into account with an R_a -factor. For the peak the results are good in the first case but deviate considerably in the second case as expected, especially for the large Peclet numbers.

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This analysis is at best a first estimate of the penetration depth. The assumed cutoff in concentration - 48 % - and the handling of the contact time is arbitrary. The effects of longitudinal dispersion to prolong and the decay to shorten the contact time are also neglected here. Therefore, another case is chosen to approach this problem and to check the previous assumptions; the case of flow through a bed with mono-sized blocks. Since, in a distribution, the smaller blocks occupy only a fraction of the total volume, the error in using an R_a -factor will be less than for the case of uniform blocks.

For uniform spherical blocks the transport equations for a single decaying species and no sorption on the external fracture surfaces, in dimensionless form, are:

$$\frac{2}{3}\frac{1}{R}\frac{\partial u_{f}}{\partial y} + \frac{\partial u_{f}}{\partial \delta} - \frac{\delta}{Pe}\frac{\partial^{2}u_{f}}{\partial \delta^{2}} = -\frac{\partial u_{p}}{\partial \rho}\Big|_{\rho=1} - \frac{\Lambda}{3R}u_{f}$$
(19)

$$2\frac{\partial u}{\partial y} = \frac{\partial^2 u}{\partial \rho^2} + \frac{2}{\rho} \frac{\partial u}{\partial \rho} - \Lambda u$$
(20)

The boundary conditions are:

when
$$\lambda = 0$$

 $u_f = 1$ $\delta = 0$ $0 < y < \Delta y$ (21a)

or when $\lambda \neq 0$

 $u_{f} = e^{-\Lambda y/2}$ $\delta = 0$ $0 < y < \Delta y$ (21b)

$$u_{f} = 0 \qquad \delta \neq \infty \qquad y > 0 \qquad (22)$$

$$u_{f} = 0$$
 $\delta > 0$ $y = 0$ (23)

$$\frac{\partial u_p}{\partial \rho}\Big|_{\rho=0} = 0 \tag{24}$$

$$u_{p} = u_{f} \qquad \rho = 1 \tag{25}$$

$$u_{p} = 0$$
 $0 < \rho < 1$ $\delta > 0$ (26)
 $y = 0$

The dimensionless quantities in equations (19) - (26) are:

$$u_{f} = C_{f}/C_{0}$$
⁽²⁷⁾

$$u_{p} = C_{p}/C_{0}$$
⁽²⁸⁾

$$\delta = \frac{3 D_{p} \varepsilon_{p}}{b^{2}} \frac{z}{mV}$$
(29)

$$Pe = \frac{zV}{D_L}$$
(30)

$$R = \frac{K}{m}$$
(31)

$$y = \frac{2 D \varepsilon_p}{K b^2} \cdot t \left(= \frac{2 t}{T}\right)^*$$
(32)

$$\rho = \frac{r}{b} \tag{33}$$

$$\Lambda = \frac{\lambda K b^2}{D_p \varepsilon_p} (= \lambda T) \star$$
(34)

*) For later reference.

The solution of these equations for u_{f} is given elsewhere (Rasmuson and Neretnieks, 1980) as

$$u_{f} = u_{f} (\delta, Pe, R, \Lambda, y)$$
(35)

For large values of R, which physically means that the accumulation capacity of the water is negligible compared to the accumulation capacity of the rock blocks of the system, the solution becomes insensitive to the values of R. In Rasmuson and Neretnieks (1981) it was shown that R has no influence if $\delta > 1$ and R > 10. This occurs when K is large, as in the case of interest here. Then (35) simplifies to:

$$u_{f} = u_{f} (\delta, Pe, \Lambda, y)$$
(36)

Another helpful variable is now introduced. This variable is related to the penetration depth in equation (18) and also to the dimensionless time y in equation (32):

$$T = K b^2 / D_p \varepsilon_p$$
(37)

We see that if the penetration depth η_e in equation (18) is equal to the radius of the sphere b then T = Δt .

We can now proceed to compare the results of the exact solution, equation (36), for a given Δt , with the results for the case where all the particles of size $b = n_e$ are in equilibrium with the flowing phase. For a stable species, $\lambda = 0$, the boundary condition (21a) gives $\Delta y =$ $\frac{2 \cdot \Delta t}{T}$ = 2. For a decaying species when we choose Δt = 3 T_{1/2}, the dimensionless decay constant Λ is obtained from equation (34) as Λ = $\lambda \cdot T = \frac{\ln 2}{T_{1/2}} \cdot 3 T_{1/2} = 3 \ln 2 = 2.0794$. Note that the parameter Λ may be regarded as a ratio of two characteristic times $\Lambda = t_{diff}/t_{dec}$, where tdiff is a characteristic time for diffusion into the rock blocks and t_{dec} is a characteristic time for radioactive decay. In chemical engineering context Λ is similar to the Thiele modulus and is a measure of the importance of diffusional resistance to the reaction in a catalyst particle. For our criterion the blocks must be fully penetrated before decay sets in. This implies that Λ must be sufficiently low or, equivalently, $T_{1/2}$ sufficiently long. With these values for Δy for the non-decaying case and Λ for the decaying plots of uf may be constructed as a function of the case dimensionless time, y, for various values of the bedlength parameter, δ, and Peclet number, Pe. The plots are normalised on the abscissa using y/δ as variable so that the breakthrough curves are always centered around the value 2/3.

These exact solution curves are compared with the case where the particles are in equilibrium. This case is described by the following relations also given in the same dimensionless form:

$$\frac{2}{3}\frac{1+R}{R}\frac{\partial u_{f}}{\partial y} + \frac{\partial u_{f}}{\partial \delta} - \frac{\delta}{Pe}\frac{\partial^{2}u_{f}}{\partial \delta^{2}} = -\frac{(1+R)\Lambda}{3R}u_{f}$$
(38)

with the same boundary conditions as before: equations (21)-(23).

The solution is well known for the non-decaying case (Lapidus and Amundson, 1952). The superposition of decay onto this solution is obvious and gives:

$$u_{f}(\delta, y) = \frac{1}{2} e^{-\Lambda y/2} \left[\text{erfc} \left(\sqrt{\frac{\delta \text{ Pe} (1+R)}{6Ry}} - \sqrt{\frac{3 \text{ Ry Pe}}{8 \delta (1+R)}} \right) + e^{\text{Pe}} \cdot \text{erfc} \left(\sqrt{\frac{\delta \text{ Pe} (1+R)}{6Ry}} + \sqrt{\frac{3 \text{ Ry Pe}}{8 \delta (1+R)}} \right) \right] (39)$$

It should be noted that the solution is dependent on δ/y only and not on δ and y separately. For large R this solution is also independent of R because $(1+R)/R \rightarrow 1$. If Pe $\rightarrow \infty$ (no longitudinal dispersion) we obtain a shock-wave arriving at the dimensionless time:

$$y = \frac{2}{3} \delta \frac{1+R}{R}$$

$$\tag{40}$$

In Figures 5-7 the results for $\delta = 10$, 100, 1000 and Pe = 2, 10, 50, ∞ for R $\rightarrow \infty$ and infinite leach time Δy are depicted for the non-decaying case. It is seen that the agreement between the two solutions ((36)

and (39) or (40)) is generally poor for $\delta = 10$ but quite good for $\delta = 1000$. However, if the contact time, Δt , in equation (18) is large enough the peak-heights may be close even for small δ 's.

In Figures 8-9, $\Delta y = 2.0$ for the non-decaying case. It is seen that for early times the agreement may be poor but that the maximum values are close. Figures 10-11 show the same results for the decaying case ($\Lambda = 3 \text{ gn } 2$) and $\Delta y = \infty$. The curves agree well at the maximum also in this case.

There is a further case of interest which lies between the decaying and the non-decaying case above. This case describes the situation where a nuclide, because of solubility limitations, is released to the flow field with a constant concentration C_0 during the time Δy (equation 21a) but decays so that the decay term in equation (19) must be included.

Rasmuson (1984) has obtained an analytical solution for this case (equations (19)-(26)) also. After long times a steady-state is obtained. It is

$$(u_{f})_{\infty} = \exp \left[\frac{1}{2} \operatorname{Pe} \left(1 - \sqrt{1 + \frac{4\delta}{\operatorname{Pe}}} \left(\frac{\Lambda}{3R} + \sqrt{\Lambda} \operatorname{coth} \sqrt{\Lambda} - 1\right)\right)\right]$$
(41)

This solution is again compared with the case where the particles are in equilibrium, equation (38). Also here a simple analytical solution has been derived (Parlange and Starr, 1978). It is:

$$u_{f}(\delta, y) = \frac{1}{2} \left\{ \exp \left[\frac{1}{2} \operatorname{Pe} \left(1 - \sqrt{1 + \frac{4}{3}} \frac{\delta \Lambda (1 + R)}{R \operatorname{Pe}} \right] \right\}$$

$$\cdot \operatorname{erfc} \left[\sqrt{\frac{\delta \operatorname{Pe} (1 + R)}{6 \operatorname{Ry}}} - \sqrt{\frac{3}{8}} \frac{\operatorname{Ry} \operatorname{Pe}}{\delta (1 + R)} + \frac{\Lambda y}{2} \right] + \frac{1}{2} \operatorname{Pe} \left(1 + \sqrt{1 + \frac{4}{3}} \frac{\delta \Lambda (1 + R)}{R \operatorname{Pe}} \right) \right] \cdot \frac{1}{2} \operatorname{erfc} \left[\sqrt{\frac{\delta \operatorname{Pe} (1 + R)}{6 \operatorname{Ry}}} + \sqrt{\frac{3}{8}} \frac{\operatorname{Ry} \operatorname{Pe}}{\delta (1 + R)} + \frac{\Lambda y}{2} \right] \right\}$$

$$\left(42 \right)$$

After long times a steady-state is obtained:

$$(u_{f})_{\infty} = \exp \left[\frac{1}{2} \operatorname{Pe} \left(1 - \sqrt{1 + \frac{4}{3} \frac{\delta \Lambda (1 + R)}{R \operatorname{Pe}}}\right)\right]$$
 (43)

For a non-decaying species $\Lambda = 0$ and equation (42) reduces to equation (39). Again for large R the solution becomes independent of this parameter. For the case of no longitudinal dispersion (Pe $\rightarrow \infty$), equation (42) simplifies to a decayed shock-wave according to:

$$u_{f} = \exp \left[-\frac{(1+R) \delta \Lambda}{3R}\right] H \left(y - \frac{2}{3} \delta \frac{1+R}{R}\right)$$
 (44)

To get an influence of the decay, Δt in equation (18) is again chosen to be 3 T_{1/2}. The results for $\delta = 10$, 100; Pe = 2, 10, 50, ∞ ; $\Lambda = 3$ In 2 and infinite leach time, $\Delta y = \infty$, are shown in Figures 12-13. Also in this case the approximation seems to be permissible. Here, we may actually obtain an exact criterion by matching the steady-states, equations (41) and (43). Using the series expansion of coth x for small x we get

$$\frac{\Lambda}{15} \ll 1 \tag{45}$$

or

$$b \ll \sqrt{15 \frac{D_p \varepsilon_p}{K} \cdot \frac{1}{\lambda}}$$
$$= \sqrt{\frac{15}{\ln 2} D_a T_{1/2}}$$
(46)

Accordingly, good agreement is obtained if Δt in equation (18) is chosen according to:

$$\Delta t << \frac{15}{\ln 2} T_{1/2}$$

The criterion used in this paper is:

$$\Delta t = 3 T_{1/2}$$

It thus can be concluded that the criteria underlying equation (18) may be used to obtain a cutoff which selects those "fines" which can be lumped into the volume fraction assumed, in the model, to be

instantaneously equilibrated. In Table 4 values of b_{cutoff} for some of the important radionuclides are given for two dissolution times, T_{1each} , 10^5 and 10^6 years and effective diffusivity $D_p \varepsilon_p =$ $5 \cdot 10^{-14}$ m²/s. The minimum of 3 $T_{1/2}$ and T_{1each} is used for Δt in equation (18) giving the lowest bound for b_{cutoff} . It is seen that b_{cutoff} is on the order of millimeters - centimeters except for the highly penetrating I-129 (due to its low sorption capacity). Due to the relatively low K-values of Sr-90 and Cs-137, these nuclides have the same order of b_{cutoff} as have the actinides. If we increase the effective diffusivity by a factor of 10, the values of b_{cutoff} in Table 4 are increased by a factor of $\sqrt{10} \sim 3.2$.

Nuclide	K (m ³ /m ³)	T _{1/2} (years)	b_{cutoff} (m) $\Delta t = min (3 T)$	1/2, ^T leach ⁾
			T _{leach} = 10 ⁵	10° (years)
Sr-90	10.8	28.1	3.51•10 ⁻³	$3.51 \cdot 10^{-3}$
Cs-137	135	30.2	1.03 • 10 - 3	1.03.10-3
Tc-99	135	2.12•10 ⁵	$3.42 \cdot 10^{-2}$	8.61•10 ⁻²
I-129	0.002	1.7•10 ⁷	8.87	2.81.101
U-238	1.35•104	4.51•10 ⁹	3.42 • 10 - 3	1.08.10-2
Np-237	н	2.14•10 ⁶	3.42 • 10 - 3	1.08.10-2
Pu-239	11	2.44•104	2.92•10 ⁻³	2.92•10 ⁻³
Am-243	u	7.37•10 ³	1.61.10-3	1.61 • 10 - 3
AIII-240		7.57910	1.01 10	1.01 10

Table 4. Values of b_{cutoff} for some important radionuclides for two dissolution times 10^5 and 10^6 years. D_p ϵ_p = $5 \cdot 10^{-14}$ m²/s. Sorption data from KBS (1983, Table 12-7). Returning to the block size distribution in the lineament, we predict that for Np-237 the cutoff, assuming infinite leach time, should be at blocksizes 0.054 m. This means that the 0.02 m blocks can be included in the R_a factor whereas the 0.10 m blocks must be treated rigorously. The values of δ , Pe and R for these cases are given in Table 5. The R_a -factor is obtained as:

$$R_{a} = 1 + \frac{K}{m} \sum_{i} F(b^{i}) = 1 + R \sum_{i} F(b^{i}) \quad up \text{ to } b^{i} = b_{cutoff} \quad (47)$$

For both cases - SMALL and LARGE - $R_a = 2.4531 \cdot 10^6$. Note that here, also for case LARGE, the smallest blocks are assumed to be equilibrated, which is a poor approximation.

<u> </u>	δ	Pe	R
SMALL	2.3426•10 ²	0.875, 21.875, ∞	2.6987•10 ⁷
LARGE	9.3703	"_	"_

Table 5. Values of dimensionless parameters in lineament problem. The δ :s are for the smallest blocks.

The results for these calculations have already been shown in Figures 3 and 4 and were seen to behave as predicted.

The discussion so far has been limited to spherical blocks. However, choosing the equivalent radius of the other shapes, to obtain the same surface-to-volume ratio, the same criteria should apply (Rasmuson, 1985a).

THE SENSITIVITY OF THE MODELLED CASES TO SOME PARAMETERS

At present there is very little data available (accessible) on the widths of lineaments and blocksize distributions within these. The investigations of 4 Swedish sites (Ahlbom et al, 1983 a-d) show that the widths of lineaments and distances between lineaments vary strongly. This is also true for the hydraulic conductivities both of the "good" rock and of the lineaments. Hydraulic calculations for these sites show that there are quantities which influence the hydraulic gradient and thus flow rate, which are subject to some variations (Carlsson et al, 1983). Other important factors subject to variations are the sorption data (Andersson et al, 1983) and matrix diffusion data (Skagius and Neretnieks, 1983). Also dispersion data are scarce and variable. The "natural" variations of the mentioned quantities are at least a factor of 2 around the mean. Usually the variations are even larger.

A simplified sensitivity analysis is presented below based on the previous examples where each of these parameters is changed, one at time, by a factor of 2 in the direction where the Np-237 release would decrease. The direction is chosen because there is a tendency in safety analysis work to choose conservative values and this approach would bring the data nearer to "best estimate" values to the parameter instead of further away. Tables 6 and 7 below define the various cases. In the example in Table 6, Pe = 0.875 for the base case, and in Table 7 it is Pe = 21.875. The analytical solution is used in the calculations and the results are presented in the last columns in the Tables as the ratio of maximum Np-237 concentration for the varied case to that for the central case. In general the peak height is more sensitive to perturbations in the input parameters for Pe = 21.875 (base case) than for Pe = 0.875 (base case). The only exception is for a variation in the Peclet-number, where we get a higher sensitivity for Pe = 0.875. This is due to the fact that dispersion plays a minor role for Pe = 21.875 and higher (compare $Pe = \infty$, Figure 4). It is seen that the sensitivity of the peak height is large for a perturbation in the water residence time, tw, but rather low for a variation in the fraction of 0.10 m blocks. However, higher sensitivity to departures in F are obtained with other block-size distributions.

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Figures 14 and 15 show the breakthrough curves for the different variations. Note that variations (3) and (4) nearly coincide except at the peak. This is to be expected since at early times an increase in either $D_{p\epsilon p}$ or K by the same constant factor has the same effect on the uptake ($\alpha \sqrt{D_{p\epsilon p} K}$). At longer times shape and size-effects become important.

		Central case	Variation		C ^{max} C ^{max} cen
Water residence time	t _w s	7.8125•10 ⁷	15.625 •107	(1)	0.35
Peclet number	Pe	0.875	1.75	(2)	0.50
Volume equilibrium constant Effective diffusivity	K m ³ /i D _p ε _p m ² /i	n ³ 1.35•10 ⁴ s 5•10 ⁻¹⁴	2.7•10 ⁴ 10•10 ⁻¹⁴	(3) (4)	0.58 0.68
Fraction of 0.10 m blocks	F(0.10)	0.0909	0.1818	(5)	0.79

Table 6. Definition of the various cases in the sensitivity analysis. The other data are as in Tables 1-2.

		(Central case	e Variatio	on	C ^{max} C ^{max} cen
Water residence time	tw	S	7.8125•10 ⁷	15.625 •10	7(1)	2.1.10-2
Peclet number	Pe		21.875	43.75	(2)	0.62
Volume equilibrium constant Effective diffusivity	K Dε	m^3/m^3 m^2/s	1.35•10 ⁴ 5•10 ⁻¹⁴	2.7•10 ⁴ 10•10 ⁻¹⁴	(3) (4)	0.13
Fraction of 0.10 m blocks	рр F(0.	10)	0.0909	0.1818	(5)	0.45

Table 7. Definition of the various cases in the sensitivity analysis. The other data are as in Tables 1-2.

DISCUSSION AND CONCLUSIONS

The PSEUDOBODY approach of lumping all different rock blocks irrespective of shape and size into blocks of a uniformly sized pseudoshape gives acceptably small errors for the cases studied if compared to the variations which must be expected due to natural variations in blocksize distribution. For the same reason, the very simple criterion for determining the blocksize, below which a more accurate resolution contributes little to the final results, seems to be a useful one. It may considerably reduce the computing effort and may also reduce the effort in the field to gather accurate information on the size-distribution of the finest fraction. For determining b_{cutoff} some additional information must, of course, be provided to define the cases of interest (which nuclides and what release time). The cutoff limit in particle size which is of interest to model "exactly" is in the range of mm to cm. The smaller sizes will influence some of the shorter lived nuclides. The longer lived actinides Np-237 and U-238, which due to solubility limitations can be expected to have long leach times, will "equilibrate" particles of cm size.

Considering the present uncertainties in determining the dispersion length (or even firmly describing the dispersion mechanisms), the accuracy of the averaging method for determining the dispersion length in a variable flow field provides some justification for using such simplifying approaches.

The very simple sensitivity analysis shows that much can be gained if field data with narrower confidence limits can be otained.

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A(x)	crossection for diffusion at distance x from block surface	L ²
a	interfacial rock surface per unit fracture volume	L - 1
Ь	block radius	L
С	concentration in water	M/L ³
Cf	concentration in water in fissures	M/L ³
С _р	concentration in water in microfissures	M/L^3
Co	inlet concentration in the water	M/L ³
D	diffusivity	L ² /T
Da	$=\frac{D_p \varepsilon_p}{K}$, apparent diffusivity in microfissures	L ² /T
DL	longitudinal dispersion coefficient	L ² /T
Dp	diffusivity in water in pores	L ² /T
F(b ⁱ)	volume fraction of blocks with radius b ⁱ	
f(x)	block size distribution	L ⁻¹
Н	Heaviside's step function	
i	hydraulic gradient	L/L
к	volume equilibrium constant	
Ka	surface distribution coefficient	L
κ _d	mass equilibrium constant	L ³ /M
m	$=\frac{\varepsilon_{f}}{1-\varepsilon_{f}}$	
Pe	$=\frac{zV}{D_L}$, Peclet number	
R	$=\frac{K}{m}$, distribution ratio	
Ra	surface retardation coefficient	
r	radial distance from center of block	L
S	reaction rate due to diffusion into block	M/L ³ T
Sk	reaction rate	M/L ³ T

Т	$= \frac{Kb^2}{D_p \varepsilon_p}$	
T _{leach}	time for dissolution of waste	Т
T _{1/2}	half life	Т
t	time	Т
∆t	contact time in equation (18)	Т
tw	water residence time	Т
uf	= C _f /C _o , dimensionless concentration in water in fissures	
$(u_f)_{\omega}$	steady state value of u _f	
up	= C _p /C _o , dimensionless concentration in water in microfissure	
٧	average velocity of water in fissures	L/T
٧ ₀	water flow rate	L ³ /L ² ,T
٧ _s	solid volume	L ³
v	velocity vector	L/T
x	radial distance from surface of block	L
У	$=\frac{2D_p\varepsilon_p}{Kb^2}t$, contact time parameter	
∆у	dimensionless time for dissolution of waste	
Z	depth below ground level	L
z	distance in flow direction	L

Greek letters

α	dispersion length	L
αf	form factor; 0, 1 and 2 for slab, cylinder and sphere, respectively	
δ	$=\frac{3D_{p}\varepsilon_{p}}{b^{2}}\frac{z}{mV}$, bed length parameter	
εf	porosity of fissures	

εp	porosity of rock matrix	
ζ	residence time, defined in equation (15)	Т
ηe	penetration depth, defined in equation (18)	L
Λ	$= \frac{\lambda \ \text{Kb}^2}{D_p \epsilon_p}$, decay parameter	
λ	decay constant of radionuclide	T-1
ρ	$=\frac{r}{b}$, dimensionless radial distance	
Ρp	density of solid rock	M/L ³

Superscript

i block size group

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*Swedish Nuclear Fuel Supply Company SKBF, Stockholm, division KBS, Technical Report No. Reports can be obtained from INIS CLEARING HOUSE, International Atomic Energy Agency, P.O. Box 100, A-1400 Vienna, Austria. Figure 1: Comparison between numerical PSEUDOBODY calculations (V = const. and V = variable respectively) with analytical solution (equation (9)) with averaged (equation (16)) Peclet number but V = const. $\alpha = 10$ m.

Figure 2: Same as Figure 1 but α = 250 m.

Figure 3: Calculations with analytical solution (equation (9)). Comparison of exact treatment of block-size distribution with solution with immediate equilibration of smallest blocks ($R_a = 2.4531 \cdot 10^6$). Data in Tables 1-2. Case "small". Pe = 0.875, 21.875 and ∞ .

Figure 4: Same as Figure 3 but Case "large".

Figure 5: Comparison of the case of instationary diffusion (equation (36)) with the case of immediate equilibration of the blocks (equations (39)-(40)) for monosized blocks. No decay and infinite leach time. Pe = 2,10,50, ∞ ; R = ∞ and δ = 10.

Figure 6: Same as Figure 5 but $\delta = 10^2$.

Figure 7: Same as Figure 5 but $\delta = 10^3$.

Figure 8: Same as Figure 5 but finite leach time $\Delta y = 2.0$.

Figure 9: Same as Figure 6 but finite leach time $\Delta y = 2.0$.

Figure 10: Same as Figure 5 but decay Λ = 3 ln 2.

Figure 11: Same as Figure 6 but decay Λ = 3 ln 2.

Figure 12: Same as Figure 10 but constant source strength.

Figure 13: Same as Figure 11 but constant source strength.

Figure 14: Sensitivity analysis. Data in Table 6. Base case (0), 2 t_w (1), 2 Pe (2), 2 K (3), 2 $D_p \varepsilon_p$ (4) and 2 F (0.10) (5).

Figure 15: Sensitivity analysis. Data in Table 7. Base case (0), 2 t_w (1), 2 Pe (2), 2 K (3), 2 $D_p \varepsilon_p$ (4) and 2 F (0.10) (5).



Figure 1



Figure 2



Figure 3



Figure 4



Figure 5



Figure 6



Figure 7



Figure 8



Figure 9



Figure 10



Figure 11



Figure 12



Figure 13



Figure 14



Figure 15

List of Technical Reports

1977–78 TR 121 **KBS Technical Reports 1 – 120.** Summaries. Stockholm, May 1979.

1979

TR 79–28

The KBS Annual Report 1979. KBS Technical Reports 79-01 – 79-27. Summaries. Stockholm, March 1980.

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1984

TR 85-01

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Stockholm June 1985.

TR 85-02

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Bengt Gentzschein Eva-Lena Tullborg Swedish Geological Company Uppsala, January 1985

TR 85-03

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Kristina Skagius Ivars Neretnieks The Royal Institute of Technology Department of Chemical Engineering Stockholm, 1985-02-07

TR 85-04

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David B. Curtis New Mexico, USA, March 1985

TR 85-05

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Kristina Skagius Ivars Neretnieks The Royal Institute of Technology Department of Chemical Engineering Stockholm, 1985-04-15

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Christer Ljunggren Ove Stephansson Ove Alm Hossein Hakami Ulf Mattila Div of Rock Mechanics University of Luleå Luleå, Sweden, October 1985

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Jacob A. Marinsky, A. Mathuthu, M. Bicking and J. Ephraim State University of New York at Buffalo Buffalo, New York 14214, July 1985

TR 85-08

In situ one-year burial experiments with simulated nuclear waste glasses

Larry L Hench, Derek Spilman and T Buonaquisti College of Engineering, Univ. of Florida, Gainesville, USA Alexander Lodding Chalmers Univ. of Technology, Gothenburg, Sweden Lars Werme SKB, Stockholm, Sweden

TR 85-09

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Björn Sundblad, Ove Landström, Rune Axelsson Studsvik Energiteknik AB, Nyköping, Sweden

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Bertrand Fritz and Marie Kam Université Louis Pasteur de Strasbourg, Institut de Géologie, France July 1985

TR 85-11

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John Smellie, Nils-Åke Larsson Swedish Geological Company, Uppsala, Sweden Peter Wikberg Royal Institute of Technology, Stockholm Sweden Leif Carlsson Swedish Geological Company, Göteborg, Sweden November 1985

TR 85-12

Hydrogeological investigations and tracer tests in a well-defined rock mass in the Stripa mine

Peter Andersson Carl-Erik Klockars Swedish Geological Company Division of Engineering Geology Uppsala 1985-11-29

TR 85-13

Analysis of hydrodynamic dispersion in discrete fracture networks using the method of moments

Anders Rasmuson Dep of Chemical Engineering, Royal Inst of Technology Stockholm June 20, 1985