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SUMMARY

Radionuclides escaping from a repository in crystalline rock for spent nuclear fuel will migrate with the seeping water in the fissures. Most radionuclides will be retarded by sorption on the rock surfaces and by diffusion into the rock matrix. Available surface for sorption and residence time are two prime variables which influence the radionuclide movement.

The water velocity may vary very much along a flow path especially if the flow path enters a strongly fissured zone (lineament).

In this paper the radionuclides in a stream tube with an arbitrary velocity along the flow path have been investigated and a numerical scheme based on the integrated finite difference method - IFDM - is proposed for practical calculations.

The transport mechanisms considered are advection and longitudinal dispersion and the retardation mechanisms used are instantaneous sorption in a portion of the rock (surface sorption) and diffusion into the rock matrix and sorption on the micropore surfaces.

An attempt is also made to account for blocks of various sizes by the MINC approach (Multiple Interacting Continua). This method accounts for the large sorption surface but small volume of small blocks and small surface area but large volume of large blocks. Any block size distribution can be handled.

1. 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 depths in crystalline rock. A typical depth considered is 500 m below the ground surface. The bedrock is fissured even at these depths and water seeps through the fissures. At larger distances - on the order of one kilometer, large 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 which are crushed to 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.

This paper sets out to investigate the impact of strongly varying velocities along the flow path. In the paper also the impact of variations in block sizes along the flow path is investigated. It is further attempted to devise a simple but for practical purposes accurate numerical scheme to calculate the nuclide movement along the whole flow path.

2. The physical situation and modelling approach

The medium consists of channels between blocks. The size of the blocks can vary along the flow path. The velocity $\bar{u}$ of the water can vary along the flow path. The radionuclides sorb reversibly on the surface of the blocks with a surface sorption coeffient K_a. They also diffuse into the blocks and sorb on their inner microfissure surfaces. The sorption on the inner surfaces is also reversible and is characterized by a linear volumetric sorption coefficient $K_d\rho$. The contact area between the fluid and the solids is a m^2/m^3 flowing water.

Figure 1 illustrates how the flow in the fissures in the rock is approximated by an equivalent homogeneous medium containing sorption surfaces.

For the flow in the z direction with cylindrical symmetry the concentration in the fluid in the fissure is described by

$$\frac{\partial c_f}{\partial t} \cdot R_a = - u_r \frac{\partial c_f}{\partial r} - u_z \frac{\partial c_f}{\partial z} + D_r \frac{1}{r} \frac{\partial}{\partial r} r \frac{\partial c_f}{\partial r} +$$

$$D_z \cdot \frac{\partial^2 c_f}{\partial z^2} - R_a \lambda c_f + a \cdot D_e \frac{\partial c_p}{\partial x}\Big|_{x=0} \qquad (1)$$

here r is the direction normal to z. D_r and D_z are the dispersion coefficients in these directions

$$R_a = 1 + a K_a \qquad (2)$$

λ is the radioactive decay constant, D_e is the effective diffusivity in the rock matrix and $\frac{\partial c_p}{\partial x}\Big|_{x=0}$ is the concentration gradient in the water in the micropores of the rock matrix at the surface of the blocks.

In the rock matrix the transport is described by $\frac{\partial c_p}{\partial t} = \frac{D_e}{R_d} \cdot \nabla^2 c_p - \lambda c_p$ which for some simple geometries can be written

$$\frac{\partial c_p}{\partial t} = \frac{D_e}{R_d} \left(\frac{\partial^2 c_p}{\partial x^2} + \frac{\beta}{x} \frac{\partial c_p}{\partial x}\right) - \lambda c_p \qquad (3)$$

$$R_d = \varepsilon_p + K_d \rho \tag{4}$$

$$c_f = c_p\big|_{r=0} \tag{5}$$

ε_p is the porosity of the rock matrix. c_p is the concentration in the micropores of the matrix. β is a factor which describes the geometry of the rock blocks. For $\beta = 0$ the blocks are infinite slabs; for $\beta = 1$ the blocks are infinite cylinders and for $\beta = 2$ they are spheres. When the penetration depth of the rock matrix is considerably smaller than the size of the block, the three geometries are equivalent.

When the concentration in the r direction is constant, the second and fourth terms in equation 1 containing derivatives of r are zero.

Assuming further that $D_z = \alpha u_z$ equation 1 simplifies to

$$\frac{\partial c_f}{\partial t} = -\frac{u_z}{R_a}\frac{\partial c_f}{\partial z} + \frac{\alpha u_z}{R_a}\frac{\partial^2 c_f}{\partial z^2}\,^{*)} - \lambda c_f + \frac{a D_e}{R_a}\frac{\partial c_p}{\partial x}\Big|_{x=0} \tag{6}$$

where $c_p\big|_{x=x_o} = c_f$.

In the formulation of equation 6 the parameters may vary with location. Equations (6) and (3) can be applied to all nuclides in a decay chain. The equations for all the daughters will have an additional term on the right hand side to account for the production from the precursor. These equations have been treated in detail in (Rasmuson and Neretnieks 1982) and are not repeated here.

The method of solution used is an integrated finite difference method (IFDM) based on the TRUMP code (Edwards 1972) which has been modified to handle chain decay and diffusion into the rock matrix. To apply the IFDM to the problem at hand where the velocity will change with

*) The third term in equation (6) is derived in the following way for the case of a varying crossection area and velocity dependent D_z

$$\frac{1}{A}\frac{\partial}{\partial z} D_z A \frac{\partial c_f}{\partial z} = \frac{1}{A}\frac{\partial}{\partial z} \alpha u_z A \frac{\partial c_f}{\partial z} = \frac{1}{A}\frac{\partial}{\partial z} \alpha Q \frac{\partial c_f}{\partial z} =$$

$$\frac{\alpha Q}{A}\frac{\partial^2 c_f}{\partial z^2} = \alpha u_z \frac{\partial^2 c_f}{\partial z^2} = D_z \frac{\partial^2 c_f}{\partial z^2}$$

distance we can design the elements such that they straddle a stream tube. The inlet and outlet surface areas are then directly obtained from the equation of continuity

$$A_i = Q/u_i \tag{7}$$

A is the crossection area of the channels.

Figure 2 illustrates the discretization along a stream tube.

As there are no radial concentration differences according to our assumption and we can neglect the concentration differences across a fissure because of the short diffusion distances in this direction we can limit the modelling to a single fissure and the rock adjacent to this fissure. Furthermore, due to symmetry it is sufficient to model only one half of the fissure. Figure 3 illustrates convergent flow in a portion of a fissure and the interaction with the adjacent rock matrix.

For fissures of equal size arranged in a cubic pattern the fissure width δ can be obtained from the block size S (fissure spacing) and the flow porosity ε_f

$$\varepsilon_f = 3\delta/(S+\delta) \text{ or neglecting } \delta$$

as $\delta \ll S$

$$\delta = S \cdot \varepsilon_f/3 \tag{8}$$

The specific surface a is

$$a = \frac{A_d}{V_f} = \frac{2}{\delta} = \frac{6}{S\varepsilon_f} \tag{9}$$

The surface retardation coefficient R_a can also be used to describe the interaction with fissure coating and filling materials which attain instantaneous and reversible equilibrium. The concept may also be applied to approximate the conditions in a crushed zone, where the particles are so small that they will be fully penetrated by the diffusing species during a time period which is short compared to the passing of the concentration pulse in the water in the fissure.

For a fissure which has a fissure filling of average thickness δ_c m with a volumetric sorption coefficient $K_{dc} \cdot \rho_c$ m^3/m^3 and a crushed zone where the fraction equilibrated is f_e, the retardation coefficient R_a is

$$R_a = 1 + \frac{\delta_c}{\delta} \cdot K_{dc}\rho_c = 1 + \frac{f_e}{\varepsilon_f} \cdot K_d\delta \qquad (10)$$

By using this formulation it is not necessary to physically model the coating in the discretization scheme.

3. Application of the integrated finite difference method IFDM to the problem

Figure 4 shows a discretization scheme along the flow path and into the rock matrix.

In the IFDM approach the discretization of equation (6) may be done by making a mass balance directly on every element. We denote the element in the fissure, on which the balance is done, by n. The coupled elements are numbered arbitrarily. In this example the upstream element is "1", the downstream element "2" and the rock matrix element is "3". Any number of elements may in principle be connected to element n.

A mass balance gives the following results

	EXCHANGED OVER SURFACE		
	A_{n1}	A_{n2}	A_{n3}
BY FLOW	$u_1 A_1 c_{n1} = Qc_{n1}$	$u_2 A_2 c_{n2} = Qc_{n2}$	-
BY DIFFUSION OR DISPERSION	$D^*_{n1}(c_1-c_n)$	$D^*_{n2}(c_2-c_n)$	$D^*_{n3}(c_3-c_n)$

LOST BY RADIOACTIVE DECAY

$$\lambda \; V_n \; c_n \; R_a$$

ACCUMULATED IN THE ELEMENT

$$R_a \; V_n \; \frac{dc_n}{dt}$$

$$D^*_{n1} = D_z \; A_{n1}/(\Delta z_{n1} + \Delta z_{1n}) \tag{11}$$

$$D^*_{n2} = D_2 \; A_{n2}/(\Delta z_{n2} + \Delta z_{2n}) \tag{12}$$

$$D^*_{n3} = A_{n3}/(\Delta x_{n3}/D_v + \Delta x_{3n}/D_e) \approx A_{n3} \; D_e/\Delta x_{3n} \tag{13}$$

A_{ni} is the surface connecting nodes n and i. c_{ni} is the concentration at the surface A_{ni}. Δx_{nk}. Δx_{kn} are the distances in elements n and k from node to surface.

D_z is the dispersion coefficient, D_e the effective diffusivity in the rock matrix and D_v the diffusivity in the water in the fissure. The dispersion coefficient D_z is assumed to be proportional to the velocity as in many other media (Fried and Combarnous 1971) with

$$D_z = \alpha \cdot u_z$$

and thus equations (11) and (12) become

$$D^*_{n1} = \alpha Q/(\Delta z_{n1} + \Delta z_{1n}) \tag{15}$$

$$D^*_{n2} = \alpha Q/(\Delta z_{n2} + \Delta z_{2n}) \tag{16}$$

The sum of all exchanges and the decay gives the accumulation in the volume V_n.

$$\underset{1}{\frac{dc_n}{dt}} = \underset{2}{\frac{Q}{V_n R_a}(c_{n1} - c_{n2})} + \underset{3}{\frac{\alpha Q(c_1 - c_n)}{V_n R_a(\Delta z_{n1}+\Delta z_{1n})} + \frac{\alpha Q(c_2 - c_n)}{V_n R_a(\Delta z_{n2}+\Delta z_{2n})}}$$

$$\underset{4}{- \lambda c_n} + \underset{5}{\frac{A_{n3} D_e}{V_n R_a \Delta x_{3n}}(c_3 - c_n)} \tag{17}$$

Equation (17) can be compared term by term with equation (6).

Term 1 is the accumulation term.

Term 2 can be transformed

$$\frac{Q}{V_n R_a}(c_{n1} - c_{n2}) = \frac{u_z \cdot A(z)\,(c_{n1} - c_{n2})}{A(z)\,R_a(\Delta z_{n1}+\Delta z_{n2})} = \frac{u_z}{R_a}\frac{\partial c}{\partial z} \quad (\text{as } \Delta z \to 0) \tag{18}$$

Terms 3 in the same way become

$$\frac{\alpha u_z}{R_a} \cdot \frac{\partial^2 c}{\partial z^2} \tag{19}$$

Term 4 is the same decay term in both equations and Term 5

$$\frac{A_{n3}}{V_n} \cdot \frac{D_e}{R_a \Delta x_{3n}} (c_3 - c_n) = \frac{a D_e}{R_a} \frac{\partial c}{\partial x}\Big|_{x=0} \quad (\text{as } \Delta x \to 0) \qquad (20)$$

Equation (17) thus is a discretized form of equation (6).

If the discretization is done by chosing volumes V_n and the relation $u = u(z)$ is known. the length of the element in the fissure can be obtained

$$\Delta z_{n1} + \Delta z_{n2} = V_n \cdot u(z)/Q \qquad (21)$$

From equation (9) the surface area for diffusion into the rock matrix can be found

$$A_d = A_{n3} = \frac{6V_n}{S \varepsilon_f} \qquad (22)$$

Equation (17) can be rewritten

$$\frac{dc_n}{dt} = \sum_k F_{nk} c_{nk} + \sum_k D_{nk} (c_k - c_n) - \lambda c_n \qquad (23)$$

where

$$F_{nk} = \frac{Q}{V_n R_a} \qquad (24)$$

$$D_{nk} = \frac{\alpha Q}{V_n R_a (\Delta z_{nk} + \Delta z_{kn})} \qquad k = 1.2 \qquad (25)$$

$$D_{nk} = \frac{A_{n3} D_e}{V_n R_a \Delta x_{kn}} = \frac{6 D_e}{S \varepsilon_f R_a \Delta x_{kn}} \qquad k = 3 \qquad (26)$$

For the elements in the matrix the same procedure can be applied. It gives

$$\frac{dc_m}{dt} = \sum_k D_{mk} (c_k - c_m) - \lambda c_m \qquad (27)$$

where $$D_{mk} = \frac{A_{mk} D_e}{V_m R_d (\Delta x_{mk} + \Delta x_{km})} \qquad (28)$$

Actually equation (23) can be applied to the elements in the matrix also by setting $F_{nk} = 0$ for the matrix elements, and using the appropriate retardation coefficient.

4. Treatment of unequal blocksizes

The previous treatment has been limited to cases where the rock blocks are of equal shape and size. They are approximated by infinite slabs or cylinders or by spheres because this simplifies the treatment of the diffusion description.

Using the IFDM approach it is fairly straightforward by an approximate method to model also a medium which consists of a multitude of different blocksizes. This has recently been demonstrated by Preuss and Narasimhan (1982) in their MINC concept. This stands for

Multiple Interacting Continua.

It is based upon the following idea adapted to the problem at hand. In a medium which consists of channels between blocks, an element of the medium can be divided into the two media, the flowing fluid and the solid blocks. In our case the fluid within an element has the same concentration. The blocks may have different concentrations at different distances from their surfaces. The species in the fluid will diffuse in (or out) of the blocks starting from the wetted surface, see figure 5. The blocks are divided into a number of shells. At the surface of the blocks, small and large alike, the fluid has the same concentration.

The first thin shell of all blocks thus reacts alike. The MINC approach assumes that all shells at the same distance from the surface behave alike in the same element of the medium. This of course is 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 ratio of $A_{i-1,i}/A_{i,i+1}$ is different.

The fluid in element m in figure 5 and the various shells of the solid can be rearranged as in figure 6 by adding all areas and volumes of the shells at a given distance from the surface.

$$A_{n-1,n}\,(x_n) = \sum_{i=1}^{N_m} A^i_{n-1,n} \tag{29}$$

where $$x_n = \sum_{j=0}^{n} d_j \tag{30}$$

N_m is the total number of blocks in element m. The fluid volume in element m is V_m

The concentration of blocks is

$$\frac{N_m}{V_m} = C_b \tag{31}$$

If the concentration of blocks and the block size distribution is constant in the medium and is independent of locus and size of V_m, ($N/V = C_b$ = constant) a more general expression for the A(x) function can be obtained.

The frequency of blocks of size S is denoted by f(S), the cross sectional area at a distance x from the surface (x=0) of the blocks within a volume V is

$$A(x) = V\, C_b \int_0^\infty f(S)\ \ A(S,x)\ dS \tag{32}$$

It is assumed that the shape is the same for all blocks so that A(S,x) is not shape dependent.

For blocks of equal size and shape f(S) = 1 for size S_0 and f(S) = 0 $S \neq S_0$. For cubes with edge length S_0 and spheres with diameter S_0 equation (32) becomes

$$A(x) = V_t(1-\varepsilon_f)\ \frac{6}{S_0}\ \left(1-\frac{2x}{S_0}\right)^2,\quad 0 < x \leq S_0/2 \tag{33}$$

For cylinders or square rods of infinite length

$$A(x) = V_t(1-\varepsilon_f)\ \frac{4}{S_0}\ \left(1-\frac{2x}{S_0}\right),\quad 0 < x \leq S_0/2 \tag{34}$$

and for infinite slabs with thickness S_0

$$A(x) = V_t(1-\varepsilon_f)\ \ \frac{2}{S_0}\qquad\qquad 0 < x \leq S_0/2 \tag{35}$$

The Figure 7 shows $A(x)/V(1-\varepsilon_f)$ for the different bodies.

Having obtained the surface area function either in diagrammatic form as in figure 6, as a discrete function, equation (29), as a continuous function, equation (32) or in the form of an A/V diagram as in figure 7 it is a straightforward matter to discretize these relations for use in an IFDM computation. The volumes of the shells are obtained directly by integration.

When the function A(x) is continuous it also may be directly used in the diffusion equation which instead of equation (3) becomes

$$\frac{\partial c}{\partial t} = \frac{1}{R_d A} \frac{\partial}{\partial x} \left(D_e A \frac{\partial c_p}{\partial x} \right) \qquad (36)$$

In equation (36) also a distance dependent diffusivity has been included.

5. Sample problem

Data from the Finnsjö site are used to examplify the use of the methods outlined in chapters 3 and 4.

5.1 The velocity along the stream tube

In figure 8 a simplified view of the bedrock surrounding a repository is shown. The stream tube which passes through a portion of the repository exits the "good" rock into the more permeable lineament. In this zone the flux is much higher and the stream tube becomes narrower. The flow of the stream tube may move in any direction including into the block of good rock on the other side of the lineament. We consider here only the case when it moves in the lineament.

The flowpaths and velocities in different stream tubes may vary considerably. Generalizations are difficult to make. We attempt here to choose a reasonable case with a bias to the conservative side for nuclide transport. It is based on the following assumptions and observations.

Assumptions: The stream tube is of constant width in the "good" rock. The hydraulic gradient i in the fissure is inversely proportional to the depth z below 25 m. Above this the gradient i is constant 0.04 m/m

$$i = 1.0 \cdot z^{-1} \qquad z > 25 \tag{37}$$

The stream tube goes straight up in the crushed rock from a level of 500 m to the surface.

Observations: The hydraulic conductivity of the rock and of the lineament can be expressed by the following relations for the Finnsjö site (Leif Carlsson personal communication 1982)

$$\text{Rock:} \qquad K_p^R = 0.013\ z^{-2.49}\ \text{m/s} \qquad z \geq 25\ \text{m} \tag{38}$$

$$\text{Lineament:} \qquad K_p^c = 0.1\ z^{-2.0}\ \text{m/s} \qquad z \geq 25\ \text{m} \tag{39}$$

The flux u_0 in the rock at 500 m depth at the Finnsjö site is 0.3 - 3 $l/m^2 \cdot$year (Carlsson and Grundfelt 1983). A central value of 1 $l/m^2 \cdot$year is chosen in the sample calculations.

Chosen data

The flowtube in the rock is 50 m long.
The flowrate in the stream tube is 1.0 l/year.
The flux in the lineament

$$u_o = Q/A = K_p^c \cdot i = 0.1 \cdot /Z/^{-3} \cdot 3.15 \cdot 10^{10}\ l/m^2 \cdot year$$

At 500 m depth this gives

u_o = 25.2 $l/m^2 \cdot$year. This is in reasonable agreement with flow data obtained in 3D flow calculations (Carlsson and Grundfelt 1983).

The flow porosity ε_f of the rock and the lineament are taken to be

Rock	10^{-4}
Lineament	$5 \cdot 10^{-4}$

For the sorbing nuclides this choice has a negligible effect as ε_f is cancelled out in the important terms in the equations (Rasmuson and Neretnieks 1981).

5.2 Block sizes

At present there are few if any data on the block size distributions. The present techniques for these measurements are based primarily on visual observations. These observations do not distinguish between fissures which carry water and those that do not. The uncertainties on the wetted block sizes are therefore fairly large at present. An attempt will still be made to asses the surface area - penetration depth relationship.

Lineaments in the Finnsjö area vary in width from 2-150 m. Within the lineaments there are crushed zones and fissured zones. There also is "good" rock adjacent to the lineament. In this case a crushed zone 0.3 m wide and a fissure zone 3 m wide is assumed. The crushed zone consists of 0.02 m "cubes", the fissure zone of 0.5 m blocks and the rock on both sides of the crushed zone has a very large extension. Figure 9 is a view over an idealized lineament.

By chosing a volume V_m so that it includes the full width of the fissured and crushed zones, and taking a height and a length equal to the blocks in the fissured zone the smallest representative volume of the crushed zone is obtained. This extends over a width of 3.3 m, is 0.5 m high and 0.5 m deep.

The crushed zone is $0.3 \cdot 0.5 \cdot 0.5$ m^3. It contains $15 \cdot 25 \cdot 25 = 9{,}375$ cubic blocks of size 0.02 m.

The fissure zone contains 6 cubic blocks of size 0.5 m.

The adjacent "good" rock contains 2 surfaces with areas 0.25 m^2 each.

Table 1 shows how the sum of the surface areas for the blocks is obtained.

Figure 10 shows the resulting A(x) relationship. Figure 11 shows A(x) for a case where the crushed zone consists of 0.1 m blocks.

It is the outermost shells of the blocks that will first be equilibrated with the nuclides carried by the flowing water. A comparison is made in table 2 of the volume available in the first 1 cm thick shell in the different cases.

The volumes available for the initial (i.e. 1 cm depth) sorption are not dramatically different for the various block sizes. If 10 cm blocks make up the crushed zone there is a volume of $128 \cdot 10^{-3}$ m^3, whereas if 2 cm blocks are available the volume increases to $166.4 \cdot 10^{-3}$ m^3.

For use in the calculations the function A(x) is most conveniently related to the fluid volume in the medium. For the lineament only the water in the zone is considered. The adjacent "good" rock is here treated as a non flow medium.

$A(x)/V_m^{fluid}$ then is

$$\frac{A(x)}{V_m^{fluid}} = A(x) \frac{1}{V_t \varepsilon_f} \qquad (40)$$

This can be utilized directly in the discretization scheme equations (26) with x=0 and equation (28).

5.3 Other data

The data in table 3 are taken from observations on the Finnsjö site (Carlsson L. 1983, Skagius and Neretnieks 1982).

Sorption data and decay constants are obtained for all nuclides individually. Some sorption data are given in table 4. They apply equally well to all fissure coating and alteration materials except for Sr and Cs on calcite. In that case K_d is an order of magnitude lower.

5.4 Discretization

The following general guidelines are used for the discretization. The volumes of the elements in the fissure are chosen either equal or in a weak geometric progression with k = 1.1 - 1.6. 10 - 20 elements in the fissure is usually sufficient. The residence volumes in the fissure are proportional to residence times as $t_n = V_n/Q$ and Q is constant. This may be directly utilized in equations 24 and 25.

The thickness of the first matrix element Δx_k adjacent to the fissure is chosen so that D_{n3} is of the same magnitude as the other small D_{nk}:s. The thickness of the matrix elements is increased by a geometric factor k between 1.1 and 1.6. Usually 5 to 10 elements are sufficient to model the diffusion in the matrix.

When there is more than one region along the flow path R_a, α, D_e, S, and ε_f may change. Then it is reasonable to choose other V and Δx_k for the discretization.

Discretization in the zones - an example

In the "good" rock 10 elements of equal volume are chosen which gives the residence times $\frac{Q}{V} = 1.57 \cdot 10^{7}$ s (0.50 years). In the lineament the the velocity is $u_f = \frac{u_o}{\varepsilon_f} = 200 \cdot Z^{-3} = -\frac{dZ}{dt}$. The residence time t_{12} between points 1 and 2 are directly obtained by integration.

$$t_{12} = -\frac{1}{200} \int_{Z_1}^{Z_2} Z^3 \, dZ = -\frac{1}{800} (Z_2^4 - Z_1^4) \qquad (41)$$

Dividing the total residence for flow from 500 m to 25 m into 10 equal parts gives the element division in table 5. The discretization constants F_{nk} and D_{nk} in the fissure elements equations (24) and (25) for the "good" rock become with α = 25 m and R_a = 1, $F_{nk} = 6.37 \cdot 10^{-8}$ S^{-1}, $D_{nk} = 3.18 \cdot 10^{-7}$ S^{-1}.

For the lineament with $R_a = 1$, $F_{nk} = 1.28 \cdot 10^{-7}\ S^{-1}$. D_{nk} for $\alpha = 250$ is given in table 5.

The discretization in the rock matrix is made with the first element having a thickness $2\Delta x_{kn}$ so that D_{nk} is of the same magnitude a the other D:s. We choose $D_{nk} = 3 \cdot 10^{-7}\ s^{-1}$ in the rock. This gives $\Delta x_{kn} = 2 \cdot 10^{-3}$ m. The following elements are obtained from the geometric series. The sum of all element lengths is half the fissure spacing (or the lesser distance needed due to smaller penetration depths)

$$S/2 = 2\Delta x_{kn}^{first} \cdot \frac{1-k^N}{1-k} \qquad (42)$$

where N is the number of elements in the block. k is the constant in the geometric progression.

6. Simplified analytical solutions

Analytical solutions are useful to check results from numeric codes. They also give an insight into the relative importance and impact of the various variables on the solution. Analytical solutions have as yet been obtained only for a few special cases of the more general problem at hand.

First a case with no dispersion is discussed in 6.1 and then in 6.2 a case with dispersion but where the dispersion effects are averaged in a certain way to allow an analytical solution to be obtained.

Two inlet boundary conditions of special interest for a repository are treated. One describes the case of congruent dissolution of a waste matrix where there is an initial inventory of a nuclide. There are no solubility limitations. This case gives a decaying step release. $c = c_0 \cdot e^{-\lambda t}$.

The second case describes a nuclide which has a solubility limitation and is released at a constant concentration. This gives a constant step release; $c = c_0$.

6.1 The case with no dispersion

With no hydrodynamic dispersion $D_z = 0$ and equation (6) becomes

$$\frac{\partial c_f}{\partial t} = - \frac{u_z}{R_a} \frac{\partial c_f}{\partial z} - \lambda c_f + \frac{a D_e}{R_a} \frac{\partial c_p}{\partial x}\Big|_{x=0} \qquad (6a)$$

$$u_z = u(z)$$

Introduce the new variable ζ

$$\zeta = \int_0^z \frac{1}{u(z)} dz \qquad u > 0 \qquad (43)$$

$$d\zeta = \frac{1}{u(z)} dz \qquad (44)$$

Substitution of dz in (6a) for $d\zeta$ results in

$$\frac{\partial c_f}{\partial t} = - \frac{1}{R_a} \frac{\partial c_f}{\partial \zeta} - \lambda c_f + \frac{a D_e}{R_a} \frac{\partial c_p}{\partial x}\Big|_{x=0} \qquad (45)$$

For initial and boundary conditions

$$
\begin{array}{llll}
c_f = c_p = 0 & t = 0 & x > 0 & z > 0 \\
c_f = c_o\, e^{-\lambda t} & z = 0 & t > 0 & (\text{or } \zeta = 0) \\
c_f = 0 & z \to \infty & t > 0 & (\zeta \to \infty) \\
c_p = 0 & x \to \infty & &
\end{array}
\qquad (46\ a\text{-}d)
$$

The last condition indicates that the rock blocks will never be fully penetrated by the nuclides.

The solution for c_f of equation (45) and (3) for $\beta = 0$ is (Neretnieks 1980).

$$c_f(z_o,t) = c_o \cdot e^{-\lambda t} \cdot \operatorname{erfc}\left\{\frac{a\sqrt{D_e R_d\ t_w}}{2\sqrt{t - R_a\ t_w}}\right\} \qquad (47)$$

where t_w is the residence time of the water in the channel from $z = 0$ to z_o. It is obtained from eq. (43)

$$t_w = \zeta_o = \int_0^{z_o} \frac{dz}{u(z)} \qquad (48)$$

For some nuclides which are retarded strongly by matrix diffusion the breakthrough times will be for $t \gg R_a\ t_w$. In such cases the water residence times per se has little influence. In equation (47) the product $a\ t_w$ can be written (equation (9) and (43))

$$at_w = \frac{6}{S\ \varepsilon_f} \int_0^{z_o} \frac{dz\ \varepsilon_f}{u_o} = \frac{6}{S} \int_0^{z_o} \frac{dz}{u_o} \qquad (49)$$

Equation (49) shows that under these conditions only the fissure spacing and the water flux influences the concentration c_f. A shorter residence time is fully compensated for by the smaller water volume in the fissure from which the nuclides diffuse into the rock matrix.

When there is no dispersion, the behaviour of migrating radionuclides are not dependent on whether the velocity is constant or not. This is also the case when the boundary condition, equation 46 b, is changed from the decaying step release to constant step release.

$$c = c_o \qquad z = 0 \qquad t > o \qquad (\text{or } \zeta = 0) \tag{50}$$

This is obtained directly from Tang et al. 1981 solution and the transform of equation (43). The full solution is not given here.

Below we compare the two parts of the stream tube defined earlier. The computation is made for neptunium -237 with $K_d\rho = 1.35 \cdot 10^4$, $T_{1/2} = 2.1 \cdot 10^6$ years. In both cases the inlet condition is taken as $c_o \cdot e^{-\lambda t}$ The argument in equation (47) is

$$\text{Arg} = \frac{a \sqrt{D_e R_d t_w}}{2 \sqrt{t - t_w R_a}} \tag{51}$$

From table 3 and equation (10) with $K_d\rho = 1.35 \cdot 10^4$ m^3/m^3. we get $R_a = 2.7 \cdot 10^6$.

As the product $a\ t_w$ is the same for both the bedrock and the crushed zone (Table 3) the difference between the migration in the two zones will be due to the difference in R_a only.

Figure 12 shows the impact of surface retardation. Surface retardation decreases the peak height by 3 orders of magnitude in this case.

For the constant step release ($c = c_o$ at $z = 0$ for $t > 0$) the steady state solution is (Neretnieks 1980).

$$c_f/c_o = e^{-t_w \left(\frac{\sqrt{D_e R_d \lambda}}{(\delta/2)} + \lambda\right)} \tag{52}$$

The retardation R_a due to surface sorption does not influence the steady state. It will, however, influence the instationary phase until steady state is reached.

With the data for plutonium the lineament and the rock will attain the same ratio of outlet to inlet concentration because t_w/δ and other data are the same.

$$c_f/c_o = 0.0824$$

As the lineament receives the fluid from the rock, the resulting outflow from the lineament is $(0.0824)^2 = c_f/c_o = 0.0068$.

6.2 Approximate analytical solution for $u = u(z)$ and $D_z > 0$

Equation (6) can be transformed using the new variable ζ (equation (43)). It becomes

$$\frac{\partial c_f}{\partial t} = -\frac{1}{R_a}\frac{\partial c_f}{\partial \zeta} + \frac{\alpha}{R_a}\frac{\partial}{\partial \zeta}\frac{1}{u}\frac{\partial c_f}{\partial \zeta} - \lambda c_f + \frac{a\,D_e}{R_a}\frac{\partial c_p}{\partial x}\bigg|_{x=0} \qquad (53)$$

If the velocity which only enters the third term is averaged in some sense to become $\bar{u}$, only the residence time ζ enters the equation.

The averaging of the velocity in the dispersion term introduces an error. Sauty (1980) has shown that for radial convergent flow where $u \propto \frac{1}{r}$ the errors are small for Pec > 3.

$$\frac{\partial c_f}{\partial t} = -\frac{1}{R_a}\frac{\partial c_f}{\partial \zeta} + \frac{\alpha}{R_a \bar{u}}\frac{\partial^2 c_f}{\partial \zeta^2} - \lambda c_f + \frac{a\,D_e}{R_a}\frac{\partial c_p}{\partial x}\bigg|_{x=0} \qquad (54)$$

Together with equation (3) and with the initial and boundary conditions

$$\begin{aligned} c_p = c_f &= 0 && t = 0 && x > 0,\ \zeta > 0 \\ c_f &= c_o\, e^{-\lambda t} && \zeta = 0 && t > 0 \\ c_f &= 0 && \zeta \to \infty && t \geq 0 \\ c_p &= 0 && x \to \infty && t \geq 0 \end{aligned} \qquad (55\ a\text{-}d)$$

the system can be solved.

The advection term, the decay term and the matrix interaction term were previously (equation (51)) shown to be dependent only on residence time and not on the distance or velocity per se. It is then possible to express $\zeta = z/\bar{u} = t_w$.

t_w is the water residence time in the fissure for flow between points z = 0 and z = z.

The solution is (Tang et al. 1981)

$$c_p/c_o = \frac{2}{\sqrt{\pi}} e^{-\lambda t} \cdot e^{\frac{1}{2} Pec} \int_{\ell}^{\infty} e^{\left(-\xi^2 - \frac{Pec}{16\xi^2}\right)} \cdot \operatorname{erfc}\left(\frac{Y}{2T}\right) d\xi \quad (56)$$

for $t > 0$ and $c_p/c_o = 0$ for $t \leq 0$

$$\ell = \frac{1}{2}\left(\frac{R_a\ Pec\ t_w}{t}\right)^{1/2} \quad (57)$$

$$Y = \frac{Pec\ t_w\ \varepsilon_p (R_d\ D_e)^{1/2}}{4\ (\delta/2)\ \xi^2} + x/\sqrt{D_a} \quad (58)$$

The concentration in the fissure c_f is obtained by setting x = 0 in equation 58 then $c_f = c_p$.

$$T = (t - R_a\ t_w\ Pec)^{1/2} \quad (59)$$

A sample calculation

Neptunium -237 migrates in the lineament. The data in table 1 are used. $K_d\delta$ for Np^{237} is 13 500 m^3/m^3. With these data the following values of the parameters in equation 56-59 are obtained.

Pec	2 and 50
R_a	$2.7 \cdot 10^6$
t_w	$7.8 \cdot 10^7$ s
R_d	13 500
D_e	$5 \cdot 10^{-14}$ m^2/s
δ	$0.083 \cdot 10^{-3}$ m

The initial and boundary conditions used imply that the concentration at the inlet is suddenly raised to c_o at time 0. It decreases with time $c_{in} = c_o \cdot e^{-\lambda t}$. This is a decaying step release.

Figure 13 shows the effluent concentration as a function of time. Three curves are shown. The curve with Pec = 50 and $R_a = 2.7 \cdot 10^6$ is similar to the curve in figure 12 with Pec = ∞ and $R_a = 2.7 \cdot 10^6$. This indicates that for Peclet numbers > 50, hydrodynamic dispersion may have a small influence when there is simultaneous diffusion into the rock matrix. A small Peclet number Pec = 2 has a very large impact on the maximum in this case, as has a lower surface retardation.

For constant step release $c = c_o$, $z = 0$, $t > 0$ the solution to equation (53) may be obtained as by Tang et al. 1981.

$$c_f/c_o = e^{\{\frac{Pec}{2z} - [(\frac{Pec}{2z})^2 + \frac{\Psi}{D_z}]^{1/2}\}z} \tag{60}$$

where

$$\Psi = R_a\lambda + \frac{(\lambda D_e R_d)^{1/2}}{\delta/2} \tag{61}$$

For the same data as previously

$c_f/c_o = 1.8 \cdot 10^{-3}$ for Pec = 50
$c_f/c_o = 0.055$ for Pec = 2.

7. IFDM calculations

In order to be able to run transport problems with variable flow and block sizes a number of modifications of the TRUMP input must be made. Details are given in Appendix 1.

All the calculations were done for Np-237 for which

$$T_{1/2} = 2.14 \cdot 10^{6} \text{ yrs}$$
$$K_d\rho = 1.35 \cdot 10^{4}$$

The data in Tables 1 and 3 were used in the calculations.

Figure 14: Variable flow, diffusion into the matrix and surface retardation.

In Figure 14 a comparison is made between numerical solutions (Pe = 50 and 500) with the analytical solution for Pe = ∞ (equation (47)). Two values of the surface retardation coefficient R_a, 1.0 and $2.7 \cdot 10^{6}$, are used. As expected the peak-height is higher for lower values of Pe. We also get an earlier breakthrough for Pe < ∞. For increasing Peclet numbers the numerical solution gets closer to the analytical one.

Figure 15: Same as Figure 14 but Pe = 2 ($R_a = 2.7 \cdot 10^{5}$ also computed). As seen the Peclet number has a large effect, as has the surface retardation. In this case there is no "exact" analytical solution. The approximate solution given by equation (56) is shown for comparison. This solution gives a later breakthrough and lower peak-height than the numerical solution. This is also the case for Pe = 50.

Figure 16: Here the block-size distribution as well as the variable velocity is taken into account. Pe = 50. MINC small is the case where the smallest particles are 2 cm. In MINC large they are 10 cm. When using the MINC approach R_a = 1.0. For t = 10^{7} years the 50 % concentration point for diffusion and sorption with constant surface concentration reaches:

$$\eta_{0.5} = 0.95 \, (D_e \, t/K_d\delta)^{\frac{1}{2}} = 3.2 \cdot 10^{-2} \text{ m.}$$

This implies that at this time point the 2 cm blocks are fully penetrated. This is not the case for the 10 cm-blocks. However. the smaller particles are more effective for adsorption due to their larger surface area.

The case with matrix diffusion and instantaneous equilibration of the smaller particles ($R_a = 2.7 \cdot 10^6$) is shown for comparison. A rather good agreement is obtained except for an earlier breakthrough in the MINC approach.

Figure 17: Same as Figure 16 but Pe = 2. Again the impact of the Peclet number is noted.

Figure 18: Here also the effect of the migration from the repository through the "solid" rock (50 m) is taken into account. Pe = 2 and the 2 cm-particles are used in the lineament. As seen the combined effect of rock and lineament lowers the peak-height with more than an order of magnitude as compared to the case with transport in the lineament only.

Figure 19: Same as Figure 17 but Q = 0.1 l/m^2,yr. This increases the residence time with a factor of 10. Approximately, the breakthrough curve will now be delayed by a factor 100 as compared to Figure 17 (see for example equation (47)). Since the curves depicted are in principle a product of the breakthrough curve without decay, with $e^{-\lambda t}$, the peak-heights are accordingly lowered.

8. Discussion and conclusions

The methods proposed here have great advantages over "exact" calculations as regards computing effort. A problem which would need rigorous three dimensional flow calculations coupled to transport calculations (also in 3D) accounting for interaction with a multitude of different sized blocks has been simplified to an equivalent one dimensional transport calculation with a solid interaction description which is no more complex than that used in interaction calculations with equally sized regularly shaped bodies (slabs, cylinders and spheres).

Such simplifications are of course bound to be less accurate than rigorous methods if such were available.

At present (1983) the description of the flow in fissured crystalline rock is less than exact due to inadequate knowledge of fissure orientation, frequency, intersections etc and the variations in these properties. We feel that the inadequacies in the proposed approach are more due to lack of data on fissure frequencies, flowrates, description of lineaments etc than on the errors introduced by the simplifications.

The proposed model indicates that the retardation in a lineament may be as important as the retardation in low permeability rock because of the larger surface areas available for sorption.

It seems warranted therefore to gather some quantitative data on lineaments. This should include data on block size distribution and data on dispersion and channeling.

9. Notation

a	specific surface	m^2/m^3
A	crossection for flow	m^2
A_d	crossection for diffusion into matrix	m^2
$A(x)$	crossection for diffusion at distance x from rock surface	m^2
$A(S,x)$	" for block of size S	m^2
c	concentration of species	mol/m^3
c_f	concentration in fluid in fissure	mol/m^3
c_p	concentration in pore water in matrix	mol/m^3
C_b	concentration of rock blocks	$number/m^3$
D_a	apparent diffusivity	m^2/s
D_e	effective diffusivity	m^2/s
D_p	pore diffusivity	m^2/s
D_v	diffusivity in water	m^2/s
D_r	dispersion coefficient normal to flow	m^2/s
D_z	dispersion coefficient in flow direction	m^2/s
D_{nk}	equation (25), (26)	s^{-1}
f_e	fraction equilibrated	
$f(S)$	frequency of blocks of size S	m^{-1}
F_{nk}	equation (24)	s^{-1}
K_a	surface equilibrium constant	m
K_d	mass equilibrium constant	m^3/kg
K_{dc}	mass equilibrium constant for coating material	m^3/kg
K_p	hydraulic conductivity	m/s
ℓ	equation (57)	-
N	number of blocks	-
Pec	Peclet number $u_f z_o/D_z$	-
Q	flow rate	m^3/s
r	radius	m
R_a	surface retardation factor	-
R_d	volume retardation factor	-
S, S_o	size of block	m
t	time	s
t_w	water residence time	s
T	equation (59)	-
u_r	water velocity in r direction	m/s
u_z	water velocity in z direction	m/s

V_f	water volume in fissures	m^3
V_n	water volume in fissures in element n	m^3
V_t	volume of water and rock	m^3
x	distance	m
Δx_{nk}	distance from node in element n to joint surface with element k	m
Y	equation (58)	-
z	distance	m
z_o	travel length	m
Δz_{nk}	as Δx_{nk}	m
Z	depth below ground level	m

Greek letters

α	dispersion length	m
β	equation (3)	-
δ	fissure width	m
δ_c	thickness of fissure filling material	m
ε_f	flow porosity	-
ε_p	matrix porosity	-
ζ	equation (43)	s
λ	decay constant	s^{-1}
ρ	density of rock	kg/m^3
ρ_c	density of fissure filling material	kg/m^3

Indices

n,m,k	number of element
nk	at interface between elements n and k

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Appendix: TRUMP input generation for transport problems with variable flow and block sizes.

The original input generation is described by Edwards (1972). The input is organized in 11 different BLOCKS. Each BLOCK supplies different information regarding the problem at hand. A summary of the BLOCK items are given in Table A1.

BLOCK	Description
1	Problem controls, limits, constants
2	Material properties
3	Reactant properties
4	Node descriptions
5	Internal diffusive connections
6	External diffusive connections
7	External concentrations (boundary nodes)
8	Variable mass-generation rates
9	Initial values of concentration, reactant concentrations, mass-generation rates
10	Flow connections
12	Nodes with properties dependent on remote concentration

Table A1: TRUMP input data blocks

In running the problems at hand, BLOCKS 3, 8, 9 and 12 are not needed. However, there are several drawbacks in the original generation of INPUT.

The first problem concerns the mesh generation. In the original TRUMP-program the only improvement, above the level where all nodes have to be specified separately, is that identical nodes may be specified on one "card" only. In the problems of concern here mesh sizes will vary widely over the discretized region. Obviously a mesh generation code is needed. The mesh generation is treated by Rasmuson and Neretnieks (unpublished manuscript) and will not be dealt with further.

Secondly, the block-size distribution according to the MINC concept has to be accounted for and the number of blocks in each flowregion will depend on the size of that region. Furthermore, flow velocity varies with the length coordinate.

It was therefore decided to write a number of programs where all this information is processed and which generates an output-file of the same format as the original INPUT to TRUMP. The following INPUT generators were written:

Program	Purpose	"Active" subroutines
ADAT	Variable velocity (lineament)	VOLX(XXX1,XXX2)
ADAT1	Variable velocity + MINC, simplified approach	AREAX(XXX), AREAY(YYY)
ADAT2	Variable velocity + MINC	VOLX(XXX1,XXX2), VOLY(YYY1,YYY2), AREAY(YYY)
ADAT3	Variable velocity + MINC + rock	"

Table A2: Input generator programs.

The "active" subroutines have the following purposes (x direction of flow, y direction into rock)

VOLX(XXX1,XXX2)

Calculates the volume available for flow according to

$$VOLX(XXX1,XXX2) = Q \int_{XXX1}^{XXX2} \frac{dx}{u(x)}$$

VOLY(YYY1,YYY2)

Calculates the specific volume of an element in the rock matrix associated with the mesh point in the fracture volume given by VOLX

$$VOLY(YYY1,YYY2) = \frac{1}{V_n} \int_{YYY1}^{YYY2} A(y)dy$$

AREAX(XXX)

Calculates interfacial areas in the flow region as

$$AREAX(XXX) = \frac{Q}{u(XXX)}$$

AREAY(YYY)

Calculates specific surface areas in the rock matrix.

$$AREAY(YYY) = \frac{A(YYY)}{V_n}$$

In practice (refer to equations (17) and (27)) we have:

Parameter	TRUMP INPUT	BLOCK
Q/R_a	FONE	1
R_a	CAPT	2
R_d	CAPT	2
αQ	CONT (area for diffusion = 1.0)	2
D_e	CONT	2
V_n	VOLX(XXX1,XXX2)	internal, 4
V_m	VOLY(YYY1,YYY2)* VOLX(XXX1,XXX2)	internal, 4
$A_{n3} = aV_n$	AREAY(0)*VOLX(XXX1,XXX2)	internal, 5
A_{mk}	AREAY(YYY)*VOLX(XXX1,XXX2)	internal, 5

Table A3: Input parameters

In the input generation program ADAT1 the volumes are approximately calculated as

$$V_n = \frac{Q\ \Delta X}{u(X_{node})} = AREAX(X_{node})\ \Delta X$$

$$V_m = a(Y_{node})\ \Delta Y\ V_n = AREAY(Y_{node})\ \Delta Y\ AREAX(X_{node})\ \Delta X$$

This approximation gives somewhat to small volumes. The approximation is good in the fissure but not so good in the rock blocks.

	0.02 m cubes	0.5 m cubes	0.25 m^2 surfaces
Number of of elements	9375	6	2
Equation for surface vs distance x per block	$6(S_o-2x)^2$	$6(S_o-2x)^2$	0.5
	$6(0.02-2x)^2$	$6(0.5-2x)^2$	0.5
Total surface vs distance	$9375 \cdot 6(0.02-2x)^2$	$6 \cdot 6(0.5-2x)^2$	0.5

Table 1. Surface areas of the different blocks in a lineament.

Block size	Number of block	Volume m^3
0.02 m	9375	$75 \cdot 10^{-3}$ a)
0.1 m	75	$36.6 \cdot 10^{-3}$ a)
0.5 m	6	$86.4 \cdot 10^{-3}$
0.25 m^2 area	2	$5 \cdot 10^{-3}$

a) Either of these make up the crushed zone.

Table 2. Volume of the first 1 cm thick shell in a volume of the lineament $0.5x0.5x3.3/(1-\varepsilon_f)$

		Rock	Lineament
Fissure spacing	S m	5	0.5
Fraction equilibrated	f_e m	-	0.1*
Diffusivity in matrix	D_e m^2/s	$5 \cdot 10^{-14}$	$5 \cdot 10^{-14}$
Total travel distance	z_o m	50	500
Dispersivity	α m	25 and 1	250 and 10
(Pec = $\frac{z_o}{\alpha}$ = 2 and 50)			
Specific surface	a $\frac{m^2}{m^3}$	$1.2 \cdot 10^4$	$2.4 \cdot 10^4$
Flux	u_o m/s	$3.15 \cdot 10^{-11}$	$0.1 \cdot z^{-3}$ (z > 25)
Residence time	t_w s	$1.57 \cdot 10^8$	$7.8 \cdot 10^7$
	a t_w $\frac{m^2 s}{m^3}$	$1.88 \cdot 10^{12}$	$1.87^{**} \cdot 10^{12}$
Fissure width	δ m	$0.167 \cdot 10^{-3}$	$0.083 \cdot 10^{-3}$

Table 3. Data for the two flow paths

* For a few hundred thousand years contact time a strongly sorbing species with $K_d\rho = 10^4$ m^3/m^3 will fully penetrate a 2 cm thick particle (Neretnieks 1980). For the contact times considered here, 2 cm particles thus can be assumed to be in "instantaneous" equilibrium and modelled as surface sorption. 0.3 m crushed zone equilibrated + 1 % of blocks gives fraction equilibrated = 0.33/3.3 = 0.1.

** The surfaces at the lineament boundaries are not included they would add 5.5 % to at_w.

		Granite	Fissure minerale	Comment
Co		0.2		
Ni		0.2		
Sr		0.004	> 0.001	
Zr		4		
Nb		4		
Tc	ox	0.0002		
	red	0.05		
I		0		
Cs		0.05	> 0.001	
Ce, Nd, Eu		> 5		
Ra		0.1		
Th		> 5		
Pa		> 5		
U	ox	0.01		U(VI)
	red	> 5		U(IV)
Np	ox	0.01		Np(V)
	red	> 5		Np(IV)
Pu	ox	3		Pu(IV)-Pu(V)
	red	> 5		Pu(III)
Am		> 5		

Table 4. K_d values (m^3/kg) for granite and fissure materials from Finnsjön. 1 week contact times in measurements. Ox and red indicate oxidizing and reducing waters respectively. (Allard 1982)

Depth Z m	Length of element m	D_{nk} s^{-1}
25.00		
	256.17	$1.25 \cdot 10^{-7}$
281.17		
	53.20	$6.02 \cdot 10^{-7}$
334.37		
	35.67	$8.97 \cdot 10^{-7}$
370.04		
	27.60	$1.16 \cdot 10^{-6}$
397.64		
	22.81	$1.40 \cdot 10^{-6}$
420.45		
	19.62	$1.61 \cdot 10^{-6}$
440.06		
	17.28	$1.85 \cdot 10^{-6}$
457.35		
	15.52	$2.06 \cdot 10^{-6}$
472.87		
	14.13	$2.26 \cdot 10^{-6}$
487.00		
	13.00	$2.46 \cdot 10^{-6}$
500.00		

Table 5. Division of elements along the lineament from 500 m depth to 25 m. Equal residence times in each element.

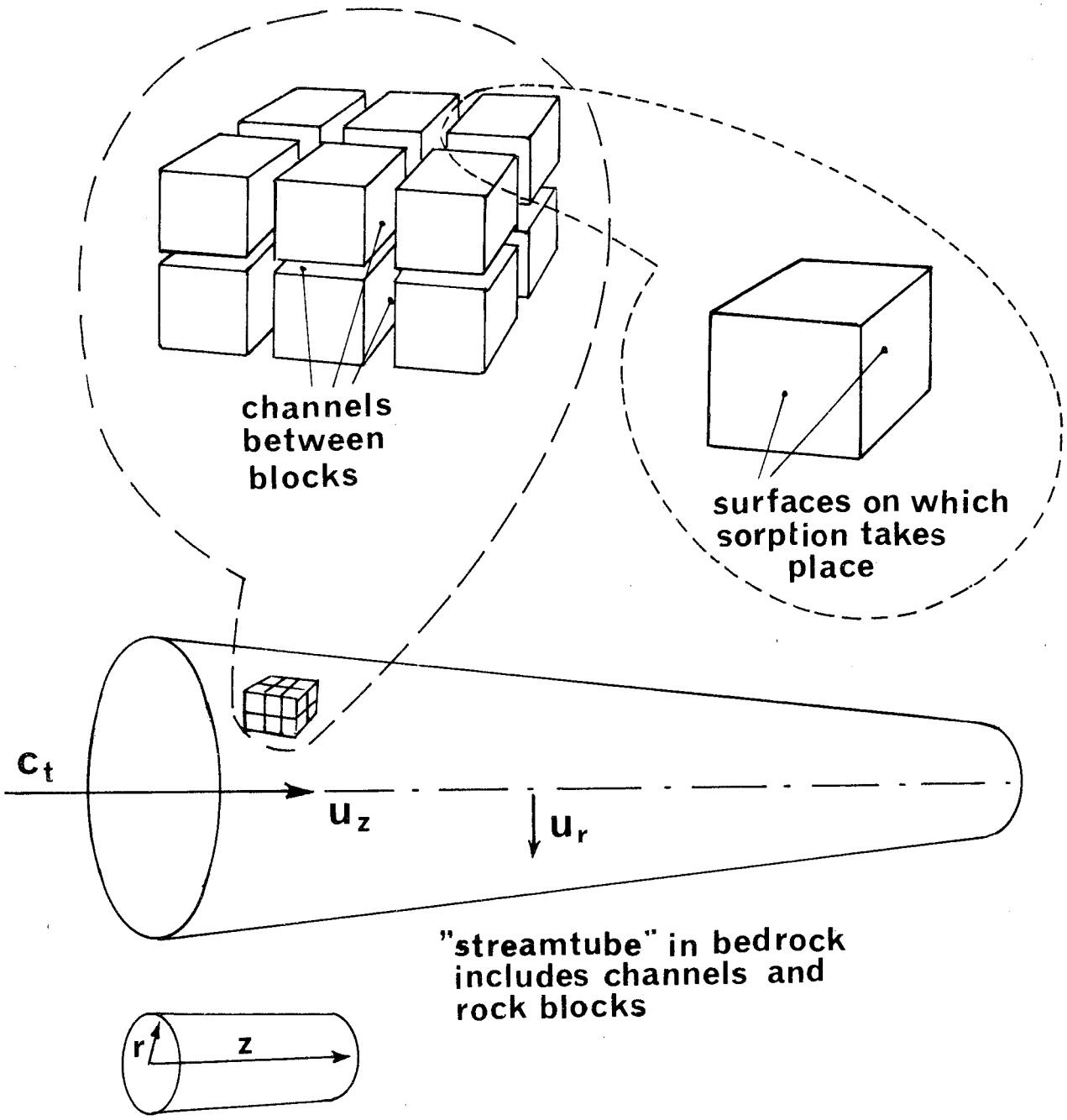

Figure 1. A simplified description of the rock.

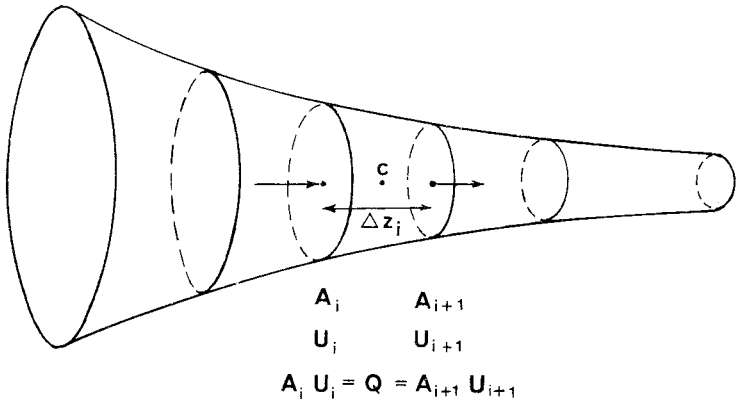

Figure 2. Discretization along a stream tube.

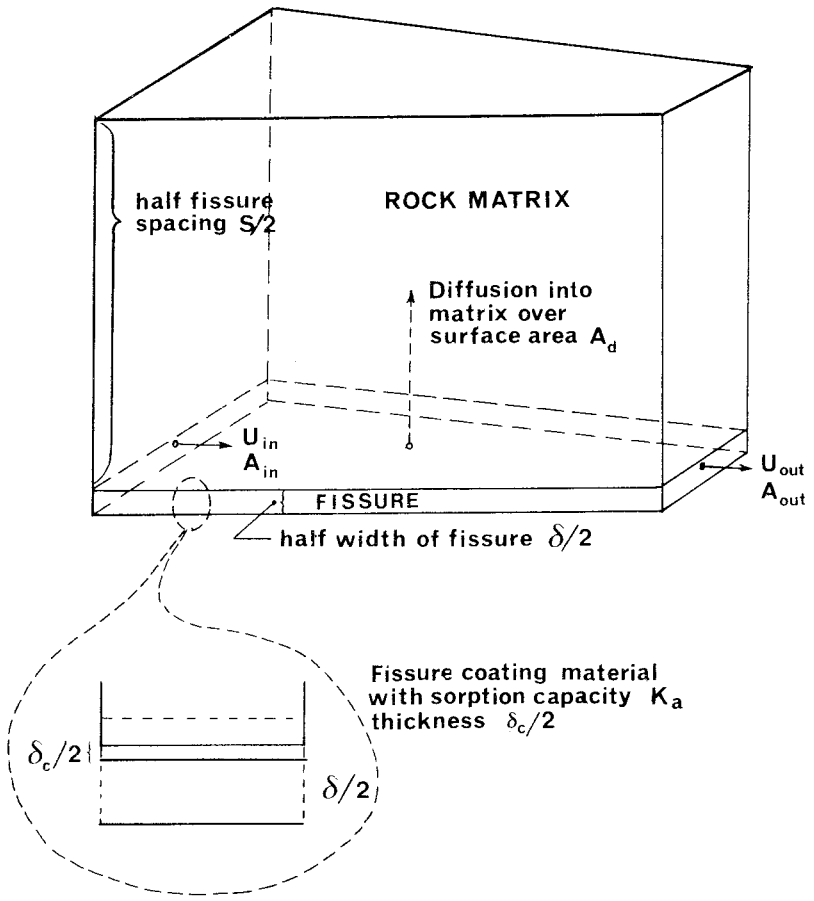

Figure 3. Simplified description of a flow channel with adjacent rock into which nuclides may diffuse.

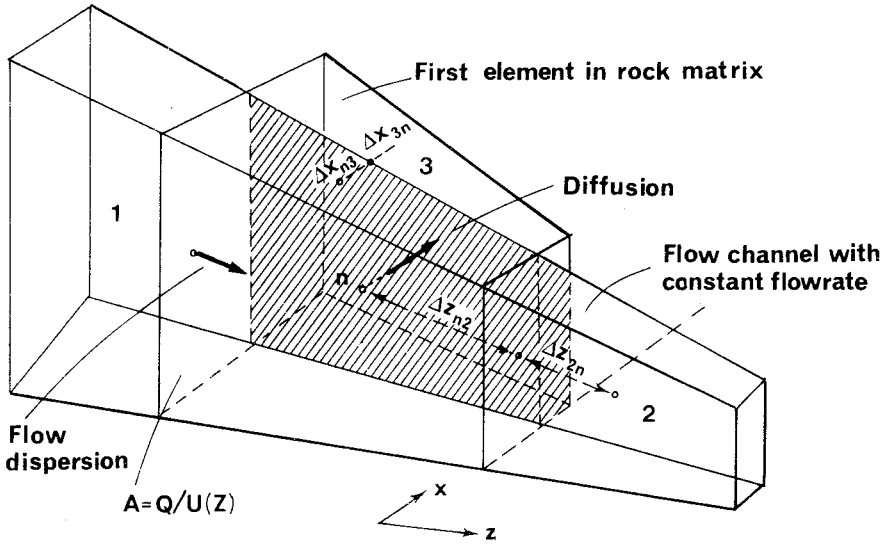

Figure 4. Discretization along a flow channel indicating the various transport modes.

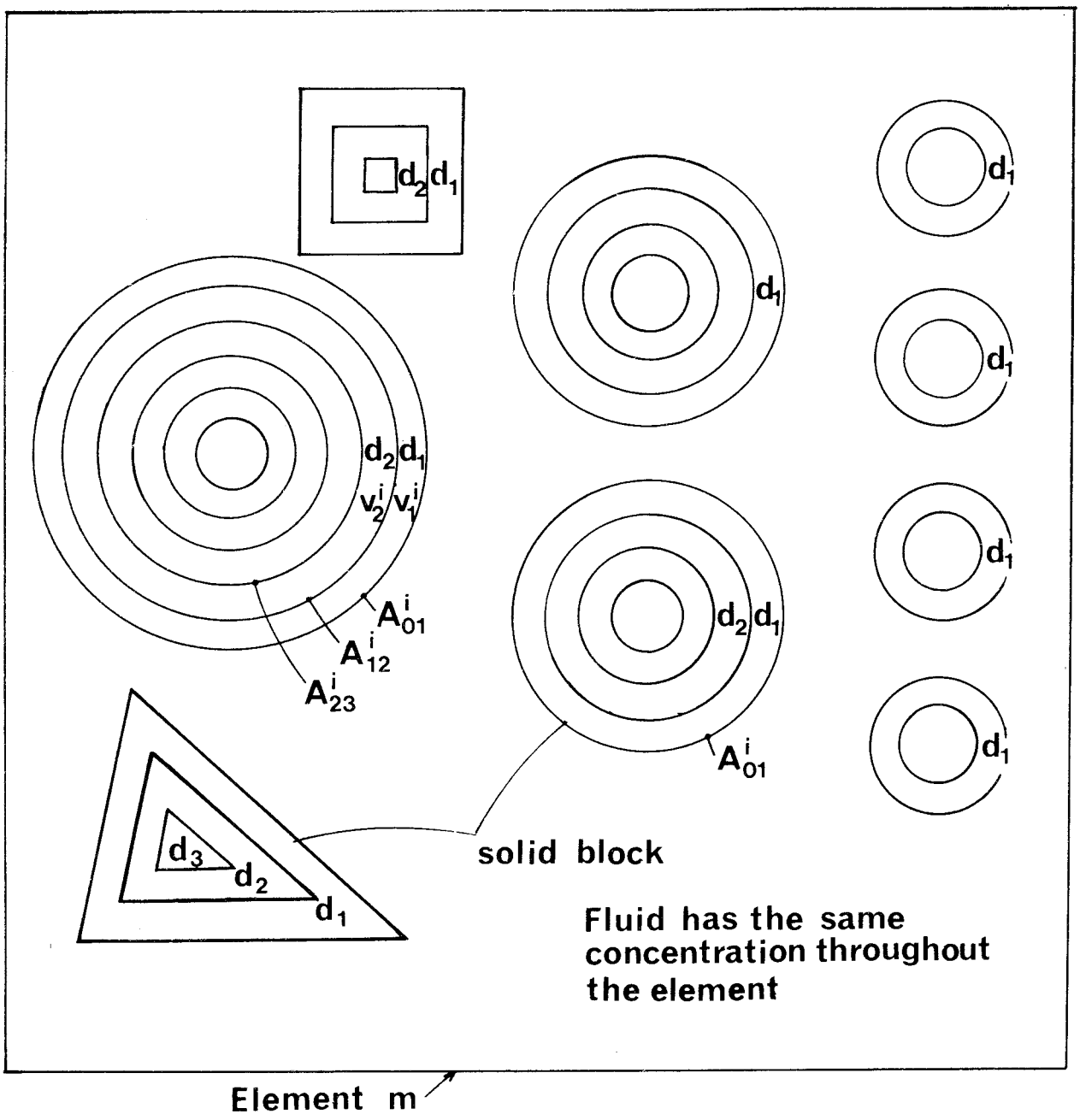

Figure 5. The principle of gathering all shells of equal distance from the surface into one volume.

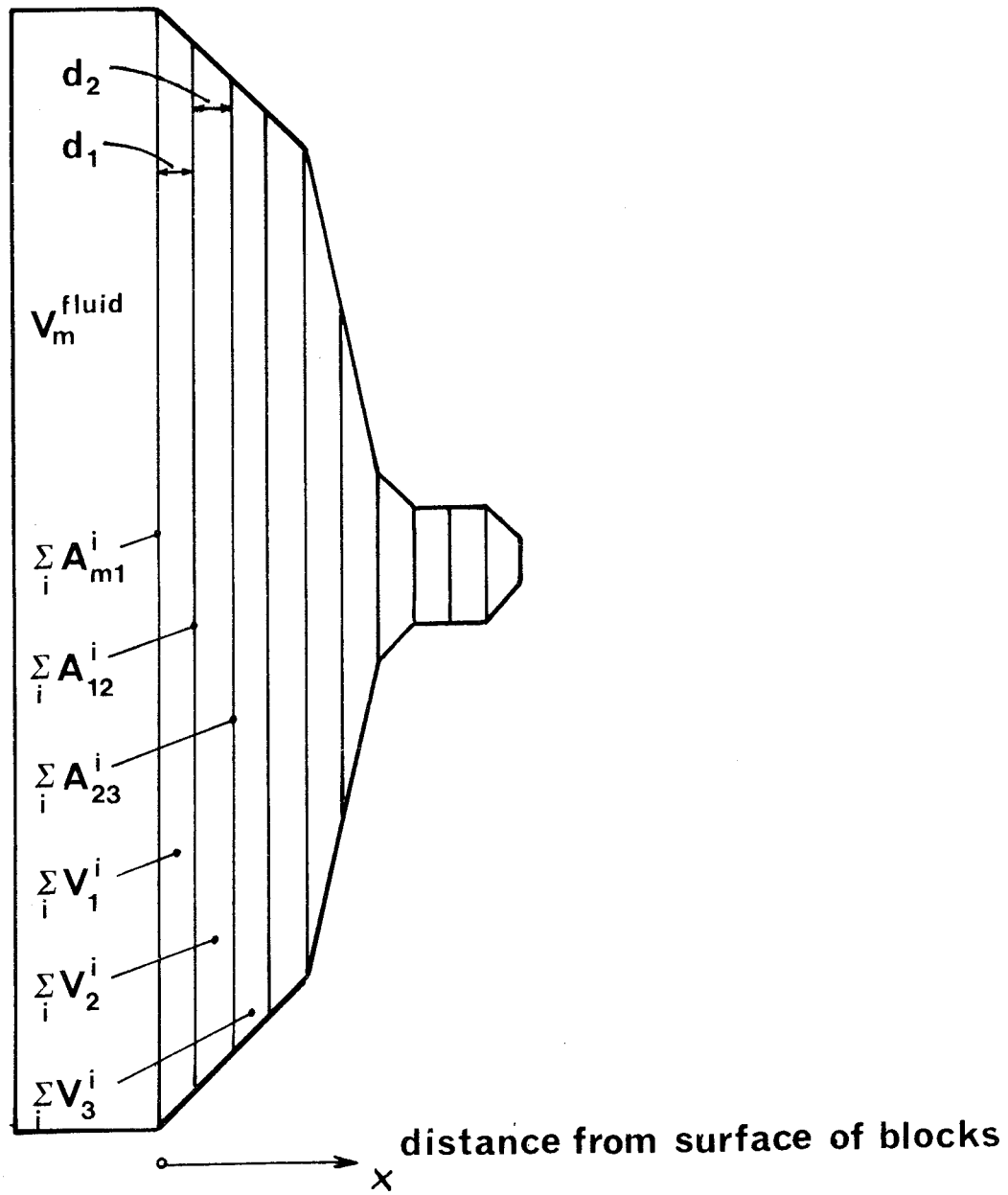

Figure 6. The sum of the areas and volumes of the blocks for various distances from the surface.

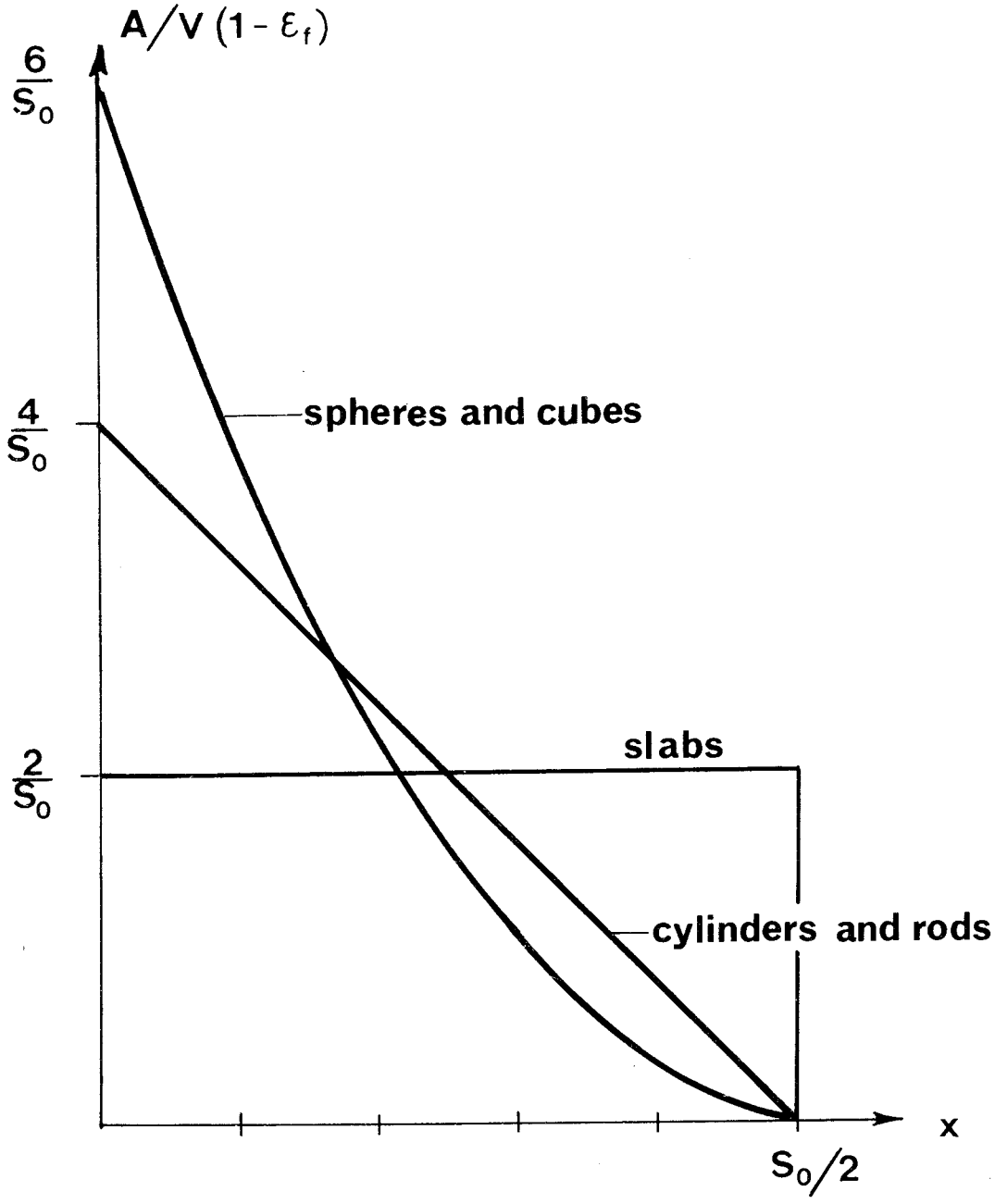

Figure 7. Area/volume functions for some regular bodies.

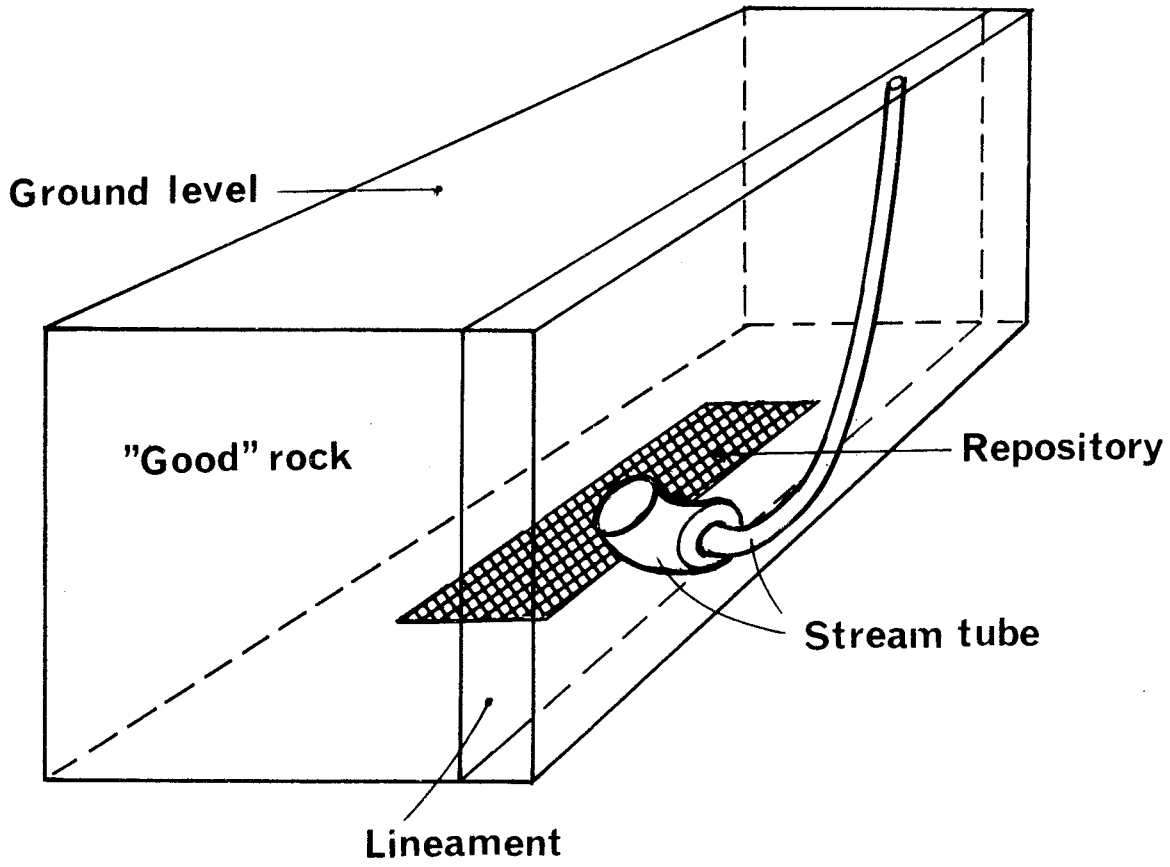

Figure 8. A simplified view over a stream tube leading from a repository to the ground.

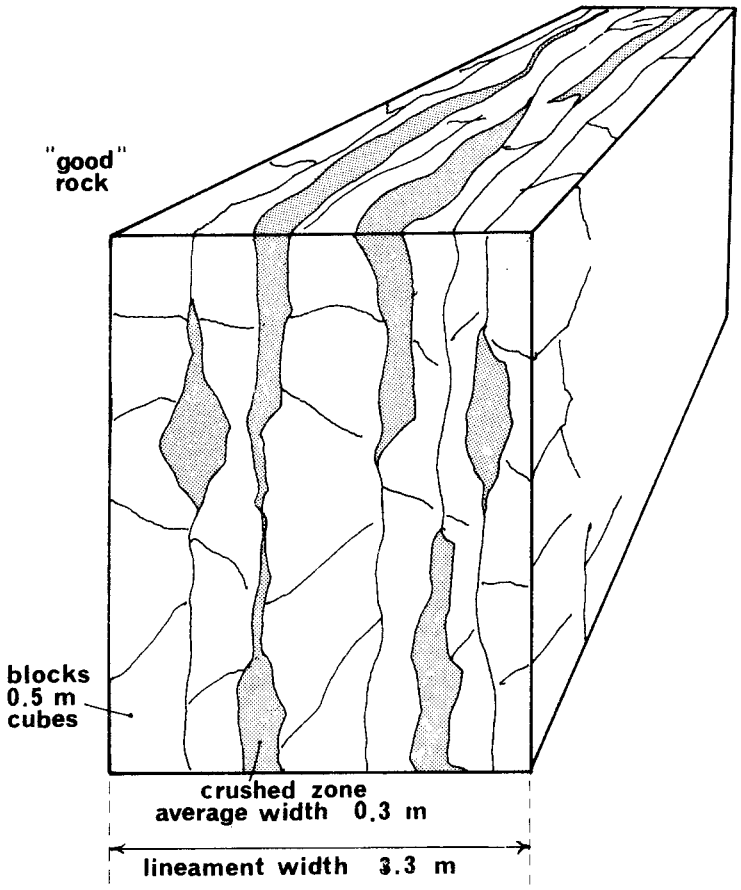

Figure 9. A lineament consisting of larger blocks interspersed with crushed zones.

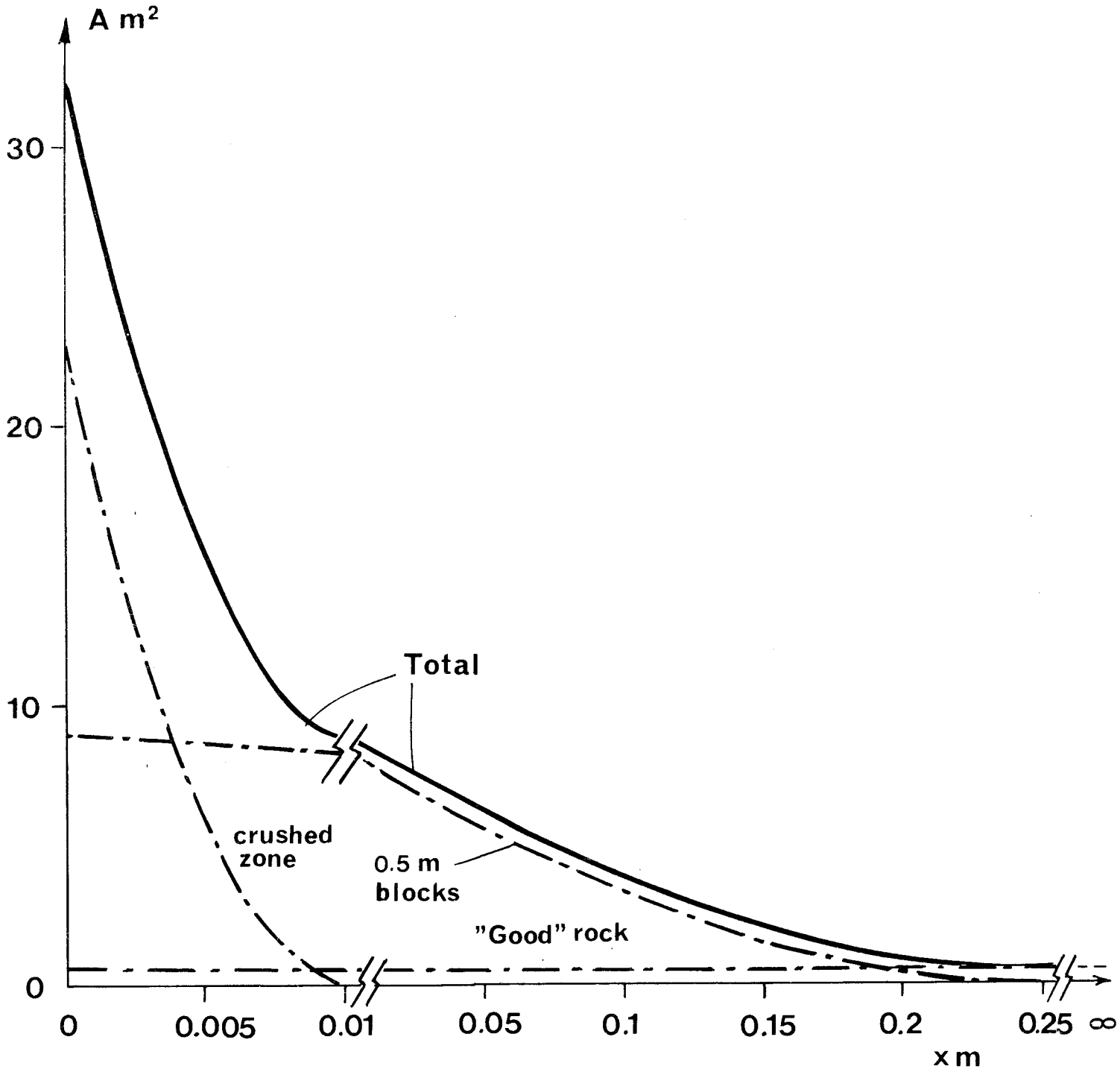

Figure 10. The area - distance function for the lineament. The area is for a 3.3x0.5x0.5 m^3 volume of the lineament - the smallest representative volume. The crushed zone consists of 0.02 m cubes.

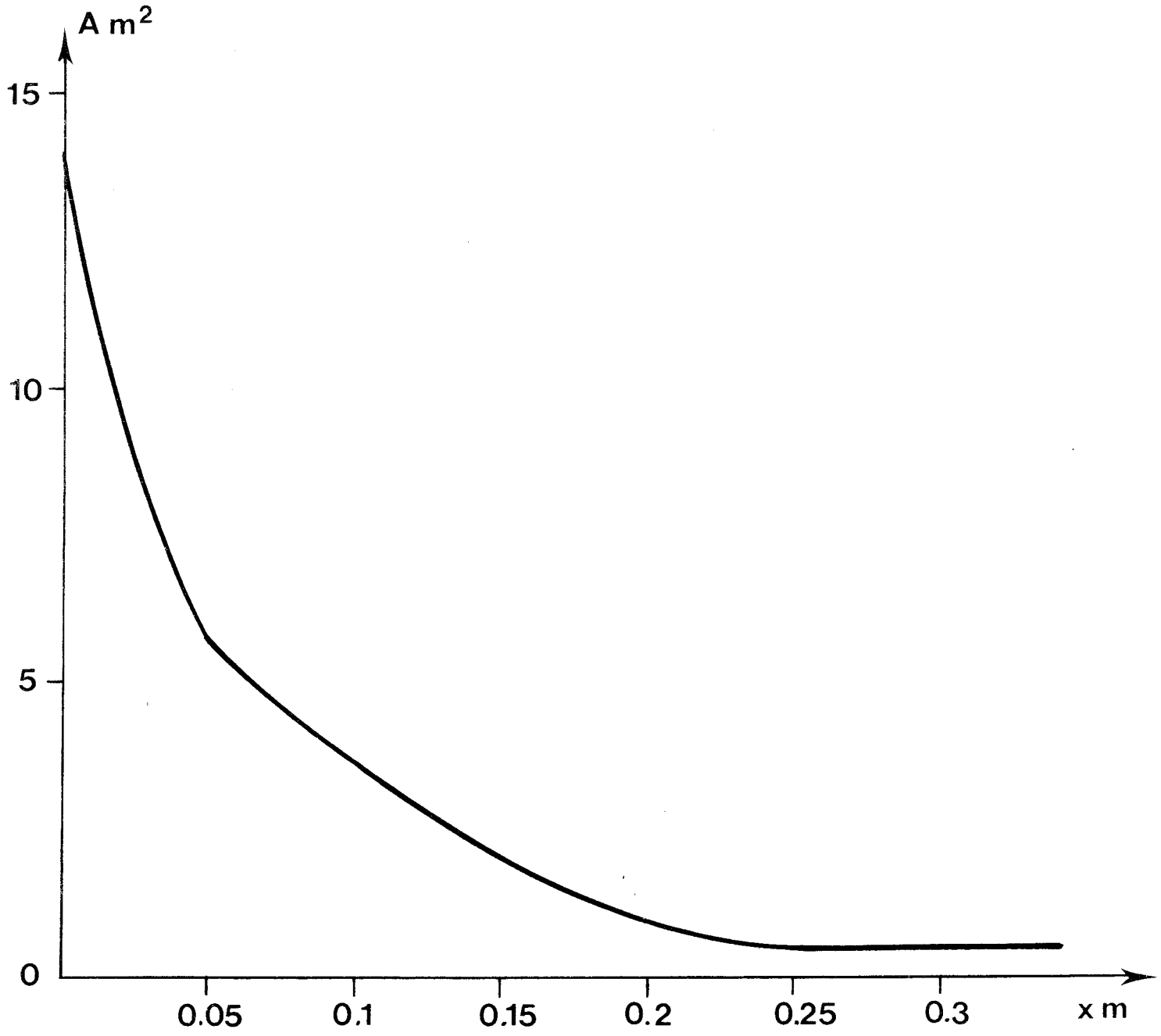

Figure 11. The same as figure 11 but with 0.1 m cubes.

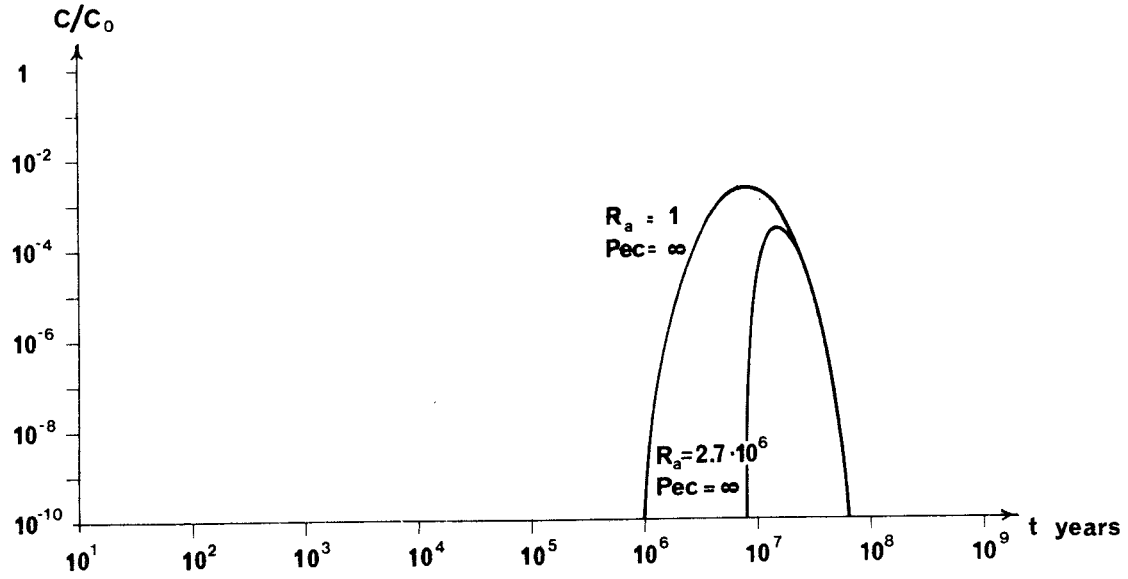

Figure 12. Results obtained from the simple analytical solution without dispersion equation 47.

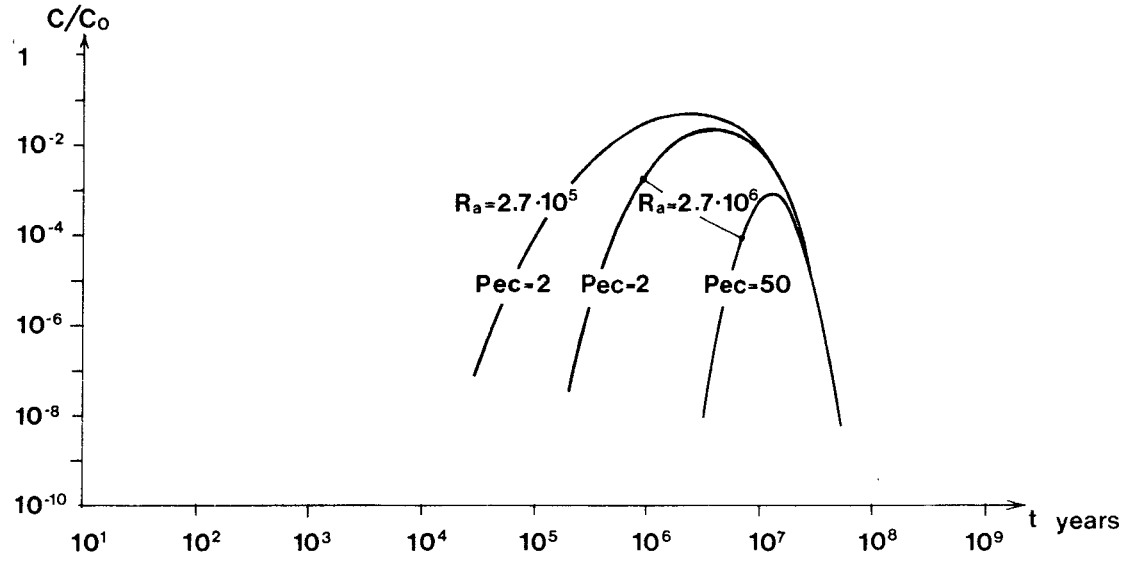

Figure 13. Results obtained from the analytical solution with dispersion equation 56.

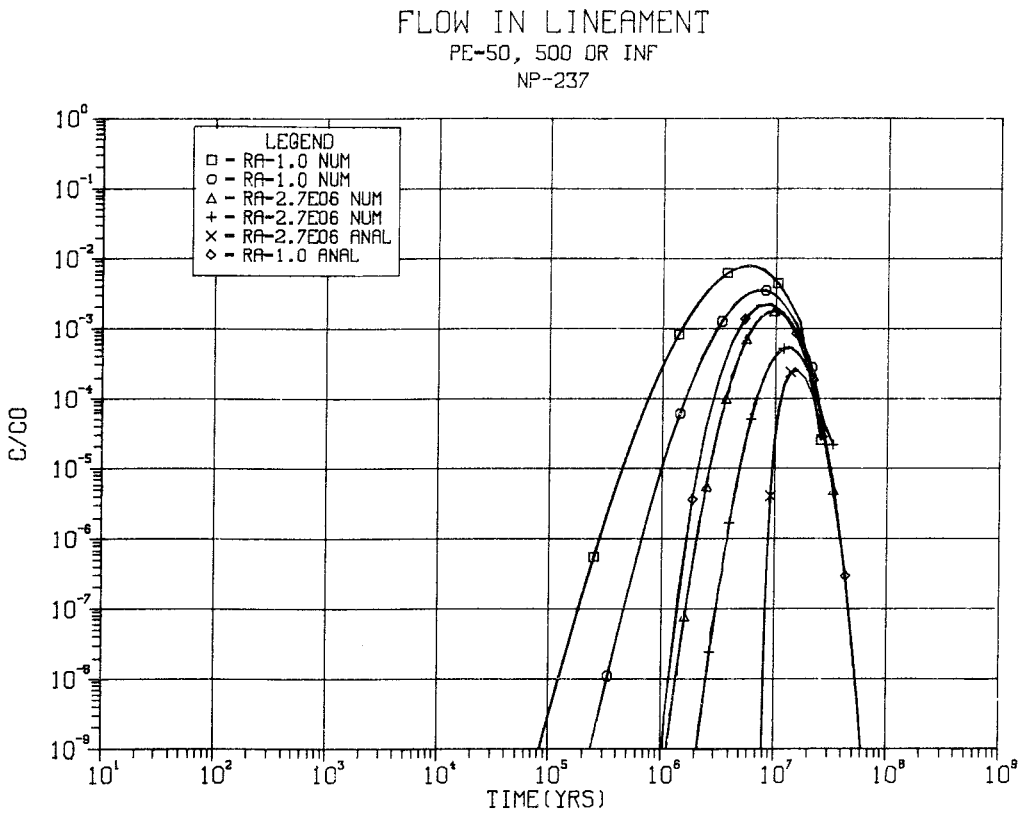

Figure 14. Comparison between numerical and analytical (Pe = ∞) solutions. Variable flow, matrix diffusion and surface retardation. The peak heights increase with decreasing Peclet numbers.

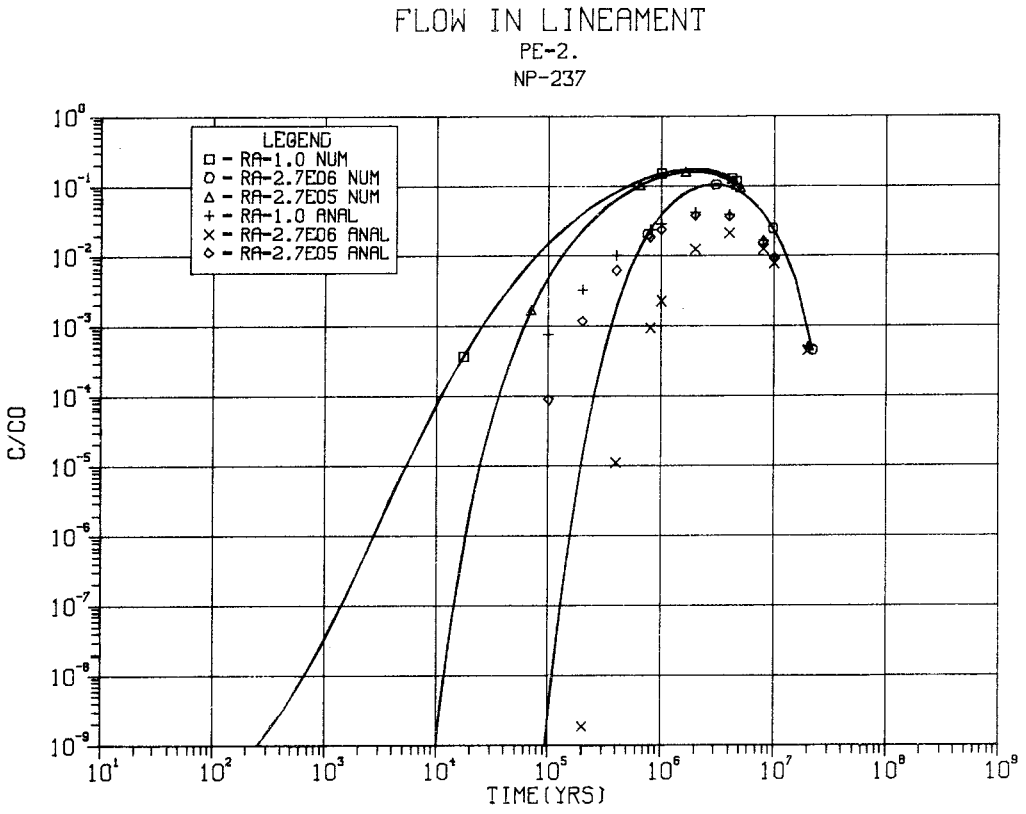

Figure 15. Comparison between numerical and analytical (Pe = 2) solutions. Variable flow, matrix diffusion and surface retardation.

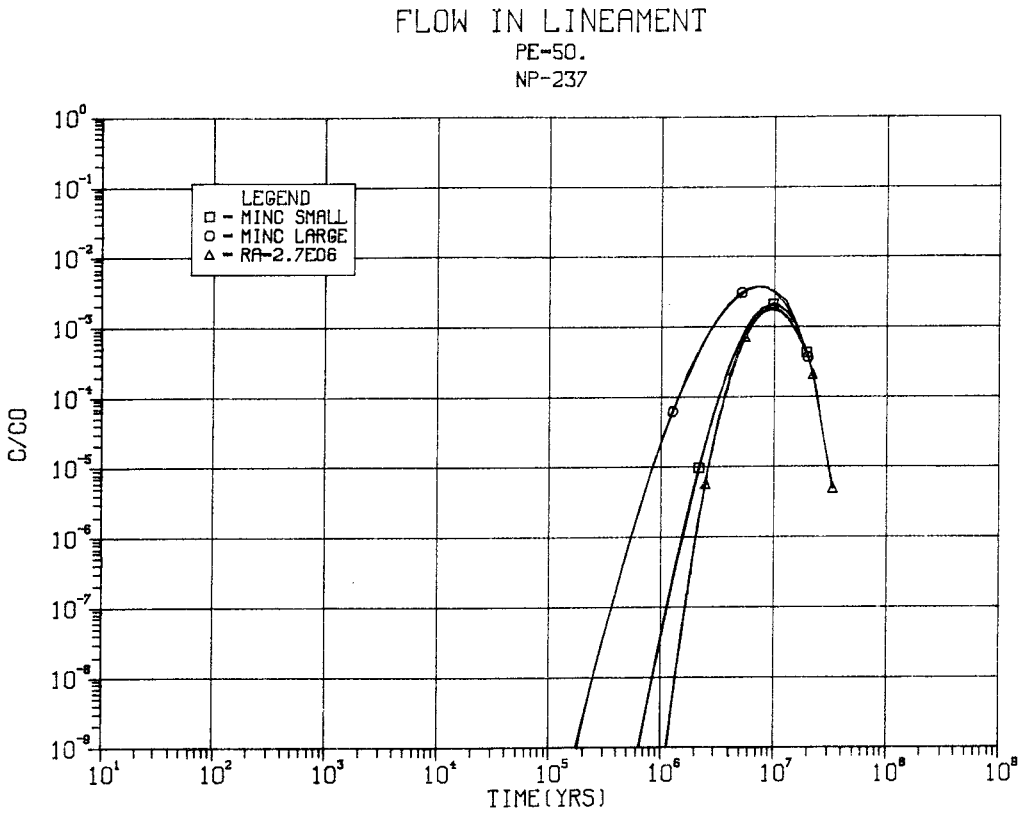

Figure 16. MINC calculations, Pe = 50. MINC SMALL = 2 cm particles. MINC LARGE = 10 cm particles. Comparison with approximate solution using surface retardation (eq. 56).

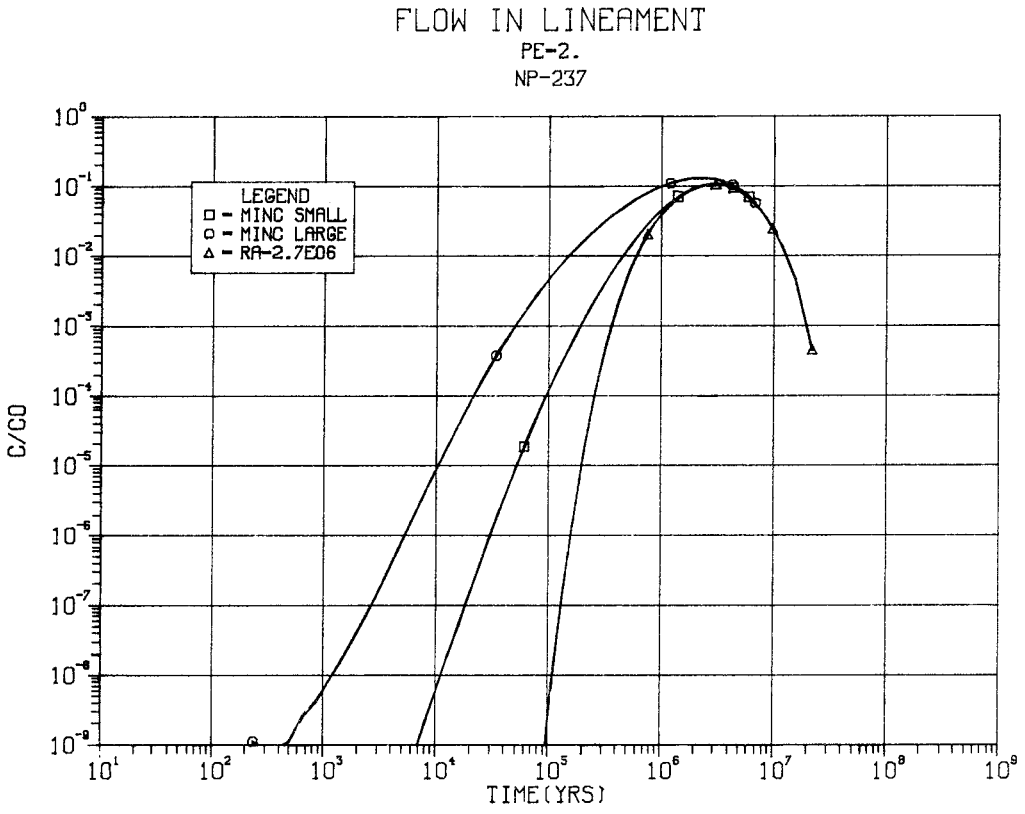

Figure 17. MINC calculations, Pe = 2.

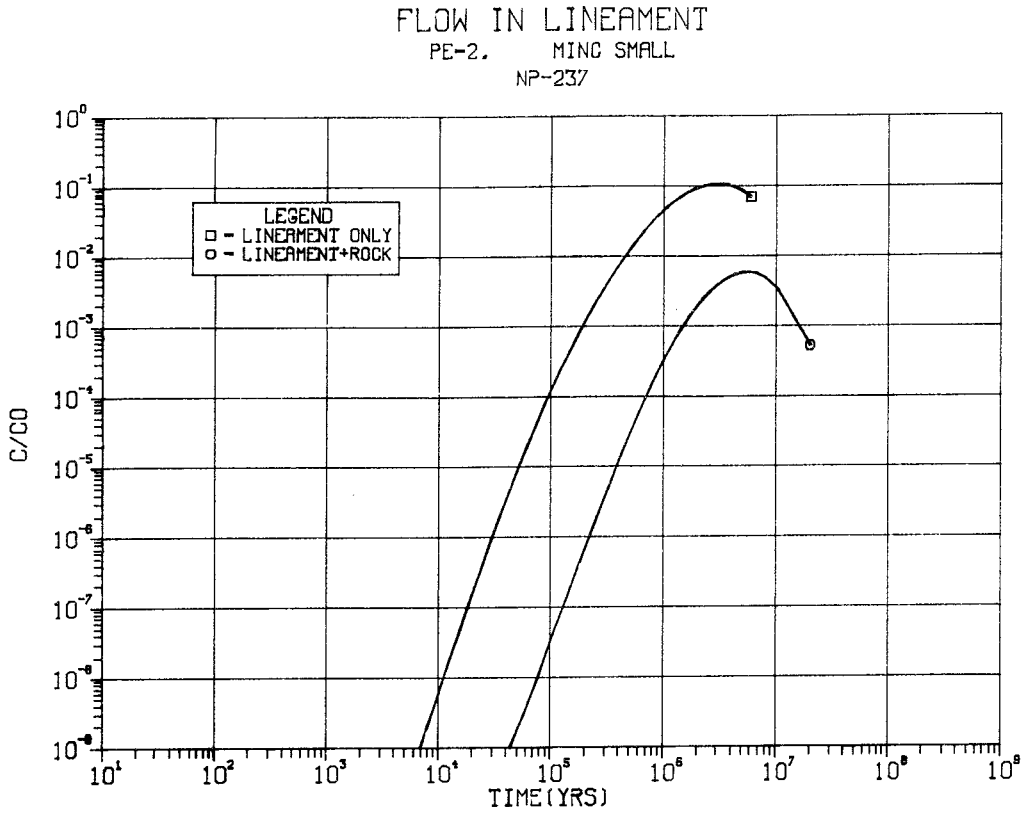

Figure 18. Comparison between flow in lineament only and 50 m rock + lineament.

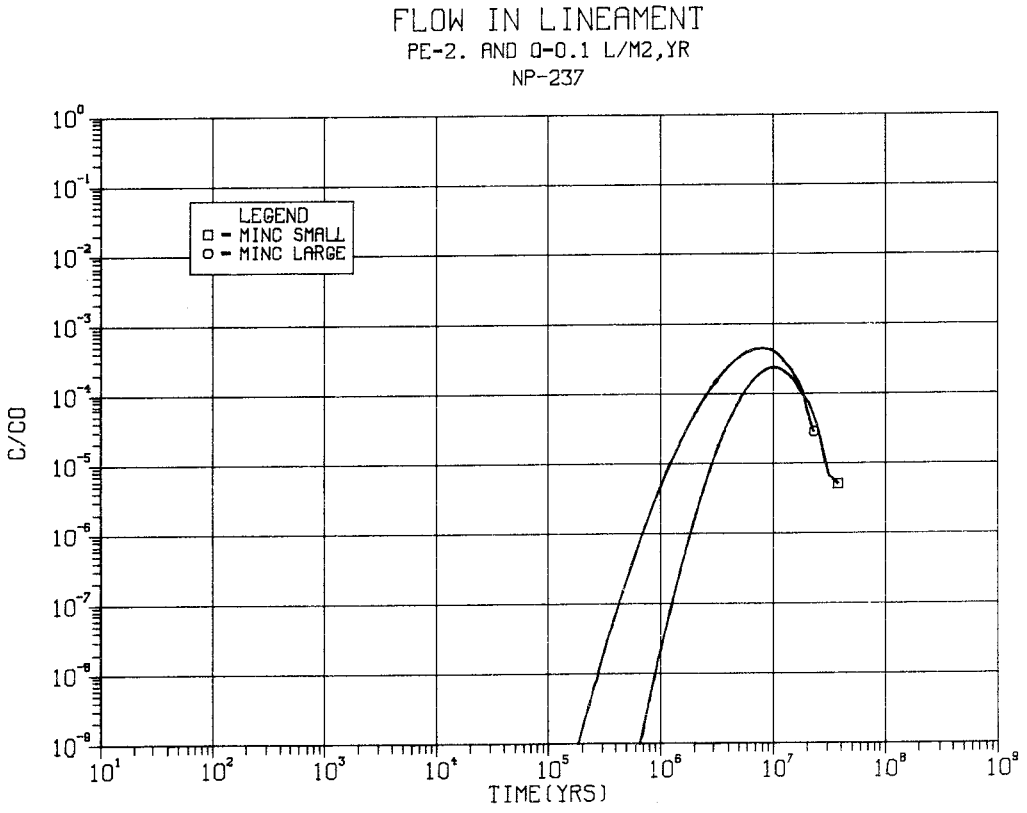

Figure 19. Same as Figure 17 but Q is ten times smaller.

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Trygve E Eriksen
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Roland Pusch
Division Soil Mechanics, University of Luleå
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University of Stockholm
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R N Parkins
University of Newcastle upon Tyne
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Alexander J Gancarz
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H Larker, ASEA
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