SKB

TECHNICAL REPORT 85-13

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

Anders Rasmuson

Dep of Chemical Engineering,
Royal Inst of Technology Stockholm

June 20,1985

SVENSK KÄRNBRÄNSLEHANTERING AB
SWEDISH NUCLEAR FUEL AND WASTE MANAGEMENT CO

BOX 5864 S-102 48 STOCKHOLM
TEL 08-67 95 40 TELEX 13108-SKB
TEL 08-665 28 00

ANALYSIS OF HYDRODYNAMIC DISPERSION IN DISCRETE FRACTURE NETWORKS USING THE METHOD OF MOMENTS

Anders Rasmuson

Department of Chemical Engineering, Royal Institute of Technology, S-100 44 Stockholm, Sweden, June 20, 1985

ANALYSIS OF HYDRODYNAMIC DISPERSION IN DISCRETE FRACTURE NETWORKS USING THE METHOD OF MOMENTS

Anders Rasmuson

July 13, 1984
Revised June 20, 1985

Department of Chemical Engineering
Royal Institute of Technology
S-100 44 STOCKHOLM
Sweden

In print in Water Resources Research (Dec. 1985)

ABSTRACT

Recent field investigations in crystalline rock give strong indications that water flows in largely isolated channels in fissured rock. The channels are located in fracture planes and may or may not connect to other channels in the same plane or at fracture intersections. In the present paper, hydrodynamic dispersion in such fracture networks is investigated using the concepts of residence time distribution (RTD) theory. It is shown that, from a set of simple relations, at least the first four statistical moments for the system response are easily obtained even for complicated networks. In particular, an equivalent dispersion coefficient may be calculated from the second central moment (variance). The effect of channeling generally decreases in systems with many mixing steps. A criterion, based on the coefficients of skewness and kurtosis, is derived for when the response of the system is in accordance with the diffusion-dispersion model. Examples show that this limit may not be obtained under realistic repository conditions in fissured rock.

CONTENTS

BACKGROUND

There are several mechanisms giving dispersion or spreading of a concentration pulse injected into a porous/fractured system: (i) molecular diffusion in the fluid, (ii) velocity variations in the fluid in a channel, (iii) velocity variations between different channels, and (iv) chemical or physical interactions with the solid material. In the following we concentrate upon the third mechanism (hereinafter denoted by hydrodynamic dispersion) which is considered to be a major cause for spreading in fissured rock.

Hydrodynamic dispersion in fissure networks is of prime importance in the calculation of radionuclide migration from a repository of spent nuclear fuel in granitic bedrock. In particular a large dispersion will cause some radioactive material to arrive earlier than the major peak and possibly there is not enough time for these radionuclides to decay to insignificant levels (Rasmuson and Neretnieks, 1981).

At the present stage it is not clear how best to describe the dispersion phenomenon in fractured rock. At one extreme there is the diffusion-dispersion model which assumes that hydrodynamic dispersion is a more or less random process similar to molecular diffusion. This model has rather successfully been used for porous media flow although it has some deficiencies like back-mixing effects (Sundaresan et al., 1980). The model predicts a dispersion coefficient which is independent of distance.

At the other extreme are the convective or channeling models (Levenspiel and Fitzgerald, 1983; Neretnieks, 1983). Here elements of fluid move past each other at a constant relative velocity with no intermediate mixing. These models predict an equivalent dispersion coefficient which increases linearly with distance.

The real case of hydrodynamic dispersion lies somewhere between these two extremes. If it lies closer to the diffusion-model or the channeling model depends upon the distance, a long travelling distance case possibly closer to diffusion-dispersion. In the present report we try to investigate this intermediate case using the concepts of residence-time-distribution (RTD) theory.

SOME FUNDAMENTAL PROPERTIES OF RESIDENCE TIME DISTRIBUTIONS

In this section we will define and develop some general properties of residence time distributions (RTD's) to be used in a subsequent discussion of RTD's in fracture networks. The content is to a considerable extent based upon the excellent monograph by Nauman and Buffham (1983).

Consider a system where the inlet concentration is given by $C_{in}(t)$ $(t > 0)$ and the outlet concentration by $C_{out}(t)$. Then:

$$C_{out}(t) = \int_0^t C_{in}(t') \, f(t-t') \, dt' =$$

$$= \int_0^t C_{in}(t-t') \, f(t') \, dt' = C_{in}(t) * f(t) \qquad (1)$$

where the symbol * denotes the convolution operation defined by either of the integrals in (1). The function f(t) is the residence time density function and f(t)dt is the probability that the residence time is in the interval (t,t+dt). Furthermore:

$$\int_0^\infty f(t) \, dt = 1 \qquad (2)$$

The Laplace transform of a convolution integral is the product of the Laplace transforms of the functions involved. Thus

$$\tilde{C}_{out}(s) = \tilde{C}_{in}(s)\ \tilde{f}(s) \qquad (3)$$

The ratio $\tilde{C}_{out}(s)/\tilde{C}_{in}(s)$ is known as the transfer function and is seen to be identical to $\tilde{f}(s)$. If $C_{in}(t) = \delta_D(t)$ (unit impulse) $C_{out}(t) = f(t)$. Thus the impulse response function is identical to the residence time density function for closed systems. By definition the system is closed if particles can make only one entrance into the system and one exit from it and the possibility of temporary excursions outside the system boundaries is not allowed.

Since f(t) is a more-or-less arbitrary function (subject only to the non-negativity and unit-area restrictions), its characterization, if not analytic, requires an infinite set of parameters. The usual choice is to characterize the distribution in terms of the moments or cumulants defined in this section. This is convenient when the distribution can be adequately (although not exactly) characterized by relatively few of these parameters. It must be stressed again that to get an exact representation of f(t) an infinite set of parameters is needed. In many cases f(t) is poorly described when only the mean residence time and variance are used.

Characterizing f(t) by its moments has the great advantage that we only need the Laplace transform $\tilde{f}(s)$ and the often difficult inversion becomes unnecessary.

The moment of order n is defined by:

$$\mu_n = \int_0^\infty t^n f(t)\, dt \qquad n = 0, 1, 2 \ldots. \tag{4}$$

These moments may be obtained from the Laplace transform $\tilde{f}(s)$ as:

$$\mu_n = (-1)^n \lim_{s \to 0} \frac{d^n \tilde{f}(s)}{ds^n} \tag{5}$$

Here

$$\mu_0 = 1$$

and

$$\bar{t} = \mu_1 = \int_0^\infty t\, f(t)\, dt \tag{6}$$

gives the mean residence time.

Special importance is attached to $\bar{t}$ since it is the average age of particles leaving the system. For incompressible fluids in closed systems, Danckwerts (1953) and Zwietering (1959) showed that:

$$\bar{t} = \frac{V}{Q} \tag{7}$$

where V is the volume of the system and Q the volumetric flow rate.

When f(t) possesses a complete set of moments, the Laplace transform can be represented as a power series in s:

$$\tilde{f}(s) = \sum_{n=0}^{\infty} \frac{(-1)^n \mu_n s^n}{n!} \tag{8}$$

where all μ_n must be finite. In principle, it is then possible to calculate f(t) by inversion of equation (8).

The central moments are defined by:

$$\mu_n' = \int_0^{\infty} (t-\bar{t})^n f(t)\, dt \tag{9}$$

We have

$$\mu_0' = \mu_0 = 1$$

$$\mu_1' = 0$$

$$\mu_2' = \mu_2 - (\bar{t})^2$$

$$\mu_3' = \mu_3 - 3\,\bar{t}\,\mu_2 + 2(\bar{t})^3 \tag{10}$$

$$\mu_4' = \mu_4 - 4\mu_3\,\bar{t} + 6\,\mu_2\,(\bar{t})^2 - 3(\bar{t})^4$$

The variance of the distribution is given by:

$$\sigma^2 = \mu_2' = \int_0^\infty (t-\bar{t})^2 f(t)\, dt = u_2 - (\bar{t})^2 \tag{11}$$

The third central moment, u_3', is known as the skewness of the distribution, and the fourth central moment, u_4', is called the kurtosis. A unimodal distribution with $u_3' < 0$ is said to be skewed to the left - that is, it has a left tailing. If $u_3' > 0$ the distribution is skewed to the right. For symmetric distributions, e.g. the Gaussian, $u_3' = 0$. The coefficient of skewness:

$$\gamma_1 = \frac{\mu_3'}{(\sigma^2)^{3/2}} \tag{12}$$

measures the skewness of the distribution relative to its degree of spread. This standardization allows us to compare the symmetry of two distributions whose scales of measurement differ. The fourth moment about the mean is related to the peakedness. The coefficient of kurtosis:

$$\gamma_2 = \frac{\mu_4'}{(\sigma^2)^2} - 3 \tag{13}$$

is a relative measure of kurtosis. The Gaussian distribution has $\gamma_2 = 0.0$, while a uniform (rectangular) distribution has $\gamma_2 = -1.2$.

The cumulants are a set of distribution characteristics related to the moments. They are defined by:

$$\kappa_n = (-1)^n \lim_{s \to o} \frac{d^n}{ds^n} [\ln \tilde{f}(s)] \tag{14}$$

The low-order cumulants are simply related to the mean and central moments of the distribution:

$$\kappa_1 = \bar{t} \qquad \kappa_3 = \mu_3'$$

$$\kappa_2 = \sigma^2 \qquad \kappa_4 = \mu_4' - 3(\sigma^2)^2 \tag{15}$$

By expanding $\ln \tilde{f}(s)$ as a power series in s, one can show formally that κ_n is the coefficient of $(-s)^n/n!$ in such an expansion, and hence that $\ln \tilde{f}(s)$ is a cumulant generating function. This can provide a very convenient means of calculating κ_n for algebraically complicated $\tilde{f}(s)$.

Complex flow networks may be synthesized by connecting simple subsystems together. The residence time distribution for the network may then be calculated from the individual distributions of the components through repeated application of equation (3).

For systems in series we obtain:

$$\tilde{C}_{out}(s) = \tilde{C}_{in}(s)\,\tilde{f}_1(s)\,\tilde{f}_2(s)\,\ldots\tilde{f}_N(s)$$

$$= \tilde{C}_{in}(s) \prod_{i=1}^{N} \tilde{f}_i(s) \tag{16}$$

and

$$\tilde{f}_s(s) = \prod_{i=1}^{N} f_i(s) \tag{17}$$

Thus the density function for the series combination is related to the density functions of the component subsystems by multiplication in the Laplace domain and by convolution in the time domain:

$$f_s(t) = f_1(t) * f_2(t) *\ldots* f_N(t) \tag{18}$$

The condition for equations (17) and (18) to hold is that the subsystems must be statistically independent so that the residence time a particle acquires in the first subsystem has no bearing on its residence time in the second one and so on.

Taking the logarithm of (17) gives:

$$\ln \tilde{f}_s(s) = \sum_{i=1}^{N} \ln \tilde{f}_i(s) \tag{19}$$

Comparison with equation (14) shows that cumulants are strictly additive for statistically independent systems in series:

$$(\kappa_n)_s = \sum_{i=1}^{N} (\kappa_n)_i \tag{20}$$

The important special cases, n = 1, 2 and 3, show that the means, variances, and skewnesses are all additive for independent systems in series.

Composite structures involving multiple flow paths can also be analyzed on the basis of equation (3), but conservation rules are now required at the junctions. Flow division points divide the volumetric flow but have no effect on particle concentrations. Flow combination points sum the incoming flows and average the incoming concentrations. These principles are illustrated in Figure 1. Application of these principles to a parallel system indicates that the composite density function for systems in parallel is a weighted sum of the component density functions in both the Laplace and time domains:

$$\tilde{f}_s(s) = \sum_{i=1}^{M} w_i \tilde{f}_i(s) \tag{21}$$

and

$$f_s(t) = \sum_{i=1}^{M} w_i f_i(t) \tag{22}$$

where w_i is the fraction of total particle flow going through subsystem "i". Comparison with equation (5) shows that for systems in parallel:

$$(\mu_n)_s = \sum_{i=1}^{M} w_i (\mu_n)_i \tag{23}$$

In particular:

$$(\mu_0)_s = \sum_{i=1}^{M} w_i = 1.0$$

$$(\mu_1)_s = \sum_{i=1}^{M} w_i (\mu_1)_i$$

$$(\mu_2)_s = \sum_{i=1}^{M} w_i (\mu_2)_i$$

Note that the variance is obtained as:

$$\sigma_s^2 = (\mu_2)_s - (\mu_1)_s^2 = \sum_{i=1}^{M} w_i (\mu_2)_i - \left[\sum_{i=1}^{M} w_i (\mu_1)_i\right]^2 \tag{24}$$

An important distinction between systems in series and in parallel, of great significance for fracture networks, is that the latter may have a variance $\sigma_s^2 > 0$ even if all $\sigma_i^2 = 0$. This is due to the fact that

dispersion in a parallel system may be caused by a distribution of retention times in the subsystems. The variance in a parallel system is zero only if:

$$\sum_{i=1}^{M} w_i(\mu_2)_i = \left[\sum_{i=1}^{M} w_i(\mu_1)_i\right]^2 \tag{25}$$

This relation is fulfilled, for example, if all w_i, $(\mu_1)_i$ and $(\mu_2)_i$ are equal.

APPLICATION TO FRACTURE NETWORKS

Water flow in fractured crystalline rock takes place in the fractures or in those parts of the fractures which are open to water flow. Several recent investigations in Sweden indicate that only a small fraction of the fractures carry water. Most fractures carry little or no water. Comparisons of the hydraulically conducting zones (from two-packer tests) and fracture maps (from core logs), have shown that only 20-50 % of all fractures carry water (KBS-3, 1983). Investigations in the Stripa mine in mid Sweden have shown that the flow in individual fractures takes place in channels (Abelin et al., 1983). These observations together with other visual observations in Stripa and other tunnels in crystalline rock support a concept of flow in fissured media which is more based on channeling than on the more often used idea of flow in a (more or less) homogeneous porous medium. The idea is that the water flows in channels which are quite widely separated and which may not for quite considerable distances intersect other channels. The channels are located in fracture planes and may or may not connect to channels in other fracture planes at fracture intersections. The connected channels may extend for considerable distances before they loose their identity by mixing with other channels.

The "fundamental" unit in the fracture networks to be considered is shown in Figure 2a. It consists of a set of parallel fractures with a common inlet and outlet. The inlet and outlet boxes are well mixed and have no volume. The fracture widths are distributed in some way given by $F(\delta_i)$ and the flow $Q(\delta_i)$ is also as function of the fracture width. As the velocity is also dependent on δ_i we get a distribution

of retention times $\Delta t(\delta_i) = \Delta t_i$. Piston flow prevails in each fracture. Here, piston flow means a uniform velocity profile, complete mixing in the radial direction and no mixing (diffusion-dispersion) in the axial direction. Such flow ensures that interconnected subsystems are statistically independent. It should be noted that Q and U in general increase with δ_i, while Δt decreases. If the cubic law applies $Q(\delta_i) \propto \delta_i^3$, $U(\delta_i) \propto \delta_i^2$ and $\Delta t(\delta_i) \propto \delta_i^{-2}$. If, on the other hand, the fractures are filled with a porous material with pores sizes $<< \delta_i$, we would have instead $Q(\delta_i) \propto \delta_i$, $U(\delta_i) =$ constant and $\Delta t_i =$ constant. In the latter case no channeling dispersion will occur. In the following we will assume that there is some dependence of Δt_i on δ_i (or on Q_i).

The fractions of particle flow are now obtained as:

$$w_i = \frac{F(\delta_i)\, Q(\delta_i)}{\sum_{i=1}^{M} F(\delta_i)\, Q(\delta_i)} = \frac{1}{\bar{Q}}\, F(\delta_i)\, Q(\delta_i) \tag{26}$$

where $\bar{Q}$ is the mean flow rate. The transfer function, its inverse and the moments, for a single channel "i", are obtained as:

$$\tilde{f}_i(s) = e^{-\Delta t_i s}$$

$$f_i(t) = \delta_D(t-\Delta t_i) \tag{27}$$

$$(\mu_n)_i = (\Delta t_i)^n$$

$$(\kappa_n)_i = \begin{cases} \Delta t_i, & n = 1 \\ 0, & n > 1 \end{cases}$$

In particular, the variance, σ_i^2, for a single channel is, of course, equal to zero. Using the relations for systems in parallel, equations (21)-(24), we obtain for the system depicted in Figure 2a:

$$\tilde{f}_s(s) = \sum_{i=1}^{M} w_i e^{-\Delta t_i s} = \frac{1}{\bar{Q}} \sum_{i=1}^{M} F(\delta_i)\, Q(\delta_i)\, e^{-\Delta t_i s}$$

$$f_s(t) = \frac{1}{\bar{Q}} \sum_{i=1}^{M} F(\delta_i)\, Q(\delta_i)\, \delta_D(t - \Delta t_i)$$

$$(\mu_n)_s = \sum_{i=1}^{M} w_i\, (\Delta t_i)^n \tag{28}$$

and

$$(\sigma^2)_s = (\mu_2)_s - (\mu_1)_s^2 = \sum_{i=1}^{M} w_i\, (\Delta t_i)^2 - \left(\sum_{i=1}^{M} w_i\, \Delta t_i\right)^2$$

Higher central moments are obtained by substitutions in equations (19). The parameter of most interest here is:

$$\left(\frac{\sigma^2}{\bar{t}^2}\right)_s = \frac{\sum_{i=1}^{M} w_i \, (\Delta t_i)^2}{\left(\sum_{i=1}^{M} w_i \, \Delta t_i\right)^2} - 1 \qquad (29)$$

If the variance of the tracer pulse at the inlet is known, the equivalent dispersion coefficient in low dispersion systems can be determined (Levenspiel, 1972) from:

$$\frac{\sigma^2_{out} - \sigma^2_{in}}{\bar{t}^2} = \frac{2D_L}{\bar{U}x} \qquad (30)$$

For the Dirac pulse at the inlet the variance is 0 and we get:

$$D_L = \left(\frac{\sigma^2}{\bar{t}^2}\right)_s \frac{1}{2} \bar{U}x \qquad (31)$$

Since $\Delta t_i \propto x$, (29) and (31) show that $D_L \propto x$ (assuming that the velocity in each channel is constant). This is to be expected since elements of fluid move past each other at constant relative velocity. Thus, the spread of fluid elements which are initially at the same position increases linearly with distance of travel. This result was also obtained by Neretnieks (1983).

It should also be noted that the derivations are equally applicable for continuous fracture width distributions. For example, the moments in equation (28) are obtained as:

$$(\mu_n)_s = \frac{\int_0^\infty f(\delta)\, Q(\delta)\, (\Delta t(\delta))^n\, d\delta}{\bar{Q}} \tag{32}$$

In the subsequent discussion the statistical properties of the "fundamental unit" (Figure 2a) will be designated by μ_1, μ_2, $\bar{t}$, σ^2, κ_n, γ_1, γ_2, D_L and L.

We now turn to the situation with N systems of the type depicted in Figure 2a in series (Figure 2b). Using equations (17) and (20) we get:

$$\tilde{f}_s(s) = \left[\frac{\sum_{i=1}^{M} F(\delta_i)\, Q(\delta_i)\, e^{-\Delta t_i s}}{\bar{Q}}\right]^N \tag{33}$$

and:

$$(\kappa_n)_s = N\, \kappa_n$$

In particular:

$$(\mu_1)s = N\, \mu_1 = N \sum_{i=1}^{M} w_i\, \Delta t_i$$

$$(\sigma^2)_s = N\, \sigma^2 = N \left[\sum_{i=1}^{M} w_i (\Delta t_i)^2 - \left(\sum_{i=1}^{M} w_i\, \Delta t_i\right)^2\right] \tag{34}$$

Accordingly:

$$\left[\frac{\sigma}{\bar{t}}\right]_s^2 = \frac{1}{N}\frac{\sigma^2}{\bar{t}^2} \tag{35}$$

and since $L_s = NL$, $(D_L)_s = D_L$ = constant as given by equation (31). Thus, the effect of channeling decreases as the fluid particles lose their identity in subsequent mixing stages. This, however, does not imply that we approach the diffusion-dispersion model already after one mixing-step. As mentioned previously the variance alone may be a poor characteristic of a distribution. We may, however, obtain a criterion, for when the diffusion-dispersion model is applicable, starting from equation (34) and comparing with a Gaussian distribution of response times. Such a distribution is obtained in the standard dispersion model at higher Peclet numbers. We would expect the system depicted in Figure 2b to give an approximately Gaussian distribution for large N because the exit age of a particle, t, is the sum of many random processes occuring in series. The central limit theorem of probability theory states that the sum of N numbers chosen from independent probability distributions will follow a Gaussian distribution in the limit as $N \to \infty$. This statement is subject only to very general conditions that are always satisfied for physically realistic processes having finite moments of all orders.

The criterion for normality may be derived by looking at higher-order moments. From equations (12)-(13) we obtain:

$$(\gamma_1)_s = \frac{(\mu_3')_s}{(\sigma_s^2)^{3/2}} = \frac{1}{\sqrt{N}}\,\gamma_1 \tag{36}$$

$$(\gamma_2)_s = \frac{(\mu_4')_s}{(\sigma_s^2)^2} - 3 = \frac{(\kappa_4)_s}{(\sigma_s^2)^2} = \frac{1}{N}\,\gamma_2 \tag{37}$$

Remember that for a Gaussian distribution $\gamma_1 = \gamma_2 = 0.0$. It is seen that, in equations (36)-(37), this limit is approached as the number of mixing stages, N, increases. According to Eadie et al (1971, p. 42) a distribution is reasonably normal if γ_1 and γ_2 are both less than 0.5. The deviations from zero for a certain N are dependent on the initial values of the skewness, γ_1, and of kurtosis γ_2. If the skewness for one mixing step is large (due to the distribution of flow and retention times) a large number of mixing steps are required to obtain a symmetric peak. This is due to the slow decrease of $(\gamma_1)_s$ ($\propto N^{-1/2}$) with N.

Consider now the system depicted in Figure 2c. What is the impact of the location (α) of the intermediate mixing step? Applying the rules given in the section on RTD-theory we get:

$$\tilde{f}_s(s) = \frac{\left(\sum_{i=1}^{M} F(\delta_i)\, Q(\delta_i)\, e^{-\alpha \Delta t_i s}\right)\left(\sum_{i=1}^{M} F(\delta_i)\, Q(\delta_i)\, e^{-(1-\alpha)\Delta t_i s}\right)}{\bar{Q}^2}$$

$$(\mu_1)_s = \sum_{i=1}^{M} w_i \alpha \Delta t_i + \sum_{i=1}^{M} w_i (1-\alpha)\, \Delta t_i = \sum_{i=1}^{M} w_i \Delta t_i = \mu_1 \qquad (38)$$

$$(\sigma^2)_s = \sum_{i=1}^{M} w_i (\alpha \Delta t_i)^2 - \left(\sum_{i=1}^{M} w_i \alpha \Delta t_i\right)^2$$

$$+ \sum_{i=1}^{M} w_i \left((1-\alpha)\Delta t_i\right)^2 - \left(\sum_{i=1}^{M} w_i (1-\alpha)\, \Delta t_i\right)^2 =$$

$$(\alpha^2 + (1-\alpha)^2) \left(\sum_{i=1}^{M} w_i\, (\Delta t_i)^2 - \left(\sum_{i=1}^{M} w_i\, \Delta t_i\right)^2\right) =$$

$$(\alpha^2 + (1-\alpha)^2)\, \sigma^2$$

Note that the intermediate step has no effect on the average residence time. Fluid particles going to faster channels after the mixing are fully balanced by particles going to slower ones. Putting $\alpha = 0$ or $\alpha = 1$ in eq. (38) gives $(\sigma^2)_s = \sigma^2$, i.e. the intermediate mixing step has no effect on the variance if it comes very early or very late. Obviously there is an intermediate position which minimizes $(\sigma^2)_s$.

Not surprisingly this minimum is obtained for $\alpha = 1/2$ giving $(\sigma^2)_{s,min} = 1/2\ \sigma^2$. In conclusion, to get miminal dispersion in the flow situation depicted in Figure 2c the mixing stages should be equally spaced.

We are now going to complicate things further and introduce a partial mixing stage as shown in Figure 2d. The system consists of a mixing stage as is shown in Figure 2c in parallel with a direct stage.

A fraction $(1-\beta)$ of the total flow Q is flowing through fractures with sizes 1 to j and fraction β through channels > j.

For the mixing stage we have:

$$\tilde{f}_s(s) = \left(\sum_{j+1}^{M} w_i' e^{-\alpha\Delta t_i s}\right)\left(\sum_{j+1}^{M} w_i' e^{-(t-\alpha)\,\Delta t_i s}\right)$$

$$(\mu_1)_s = \sum_{j+1}^{M} w_i'\,\Delta t_i$$

$$(\sigma^2)_s = (\alpha^2 + (1-\alpha)^2)\left(\sum_{j+1}^{M} w_i'\,(\Delta t_i)^2 - \left(\sum_{j+1}^{M} w_i'\,\Delta t_i\right)^2\right) \qquad (39)$$

$$(\mu_2)_s = (\sigma^2)_s + (\mu_1)_s^2$$

Here w_i' is the fraction of the total flow βQ going through the mixing stage. It is related to w_i via $w_i = \beta w_i'$. For the direct stage we get:

$$\tilde{f}_s(s) = \sum_{i=1}^{j} w_i'' \, e^{-\Delta t_i s}$$

$$(\mu_1)_s = \sum_{i=1}^{j} w_i'' \, \Delta t_i \qquad (40)$$

$$(\mu_2)_s = \sum_{i=1}^{j} w_i'' \, (\Delta t_i)^2$$

Now w_i'' is the fraction of the total flow $(1-\beta)$ Q by-passing the mixing stage and related to w_i through $w_i = (1-\beta) \, w_i''$.

Using the rules for systems in parallel we finally get:

$$\tilde{f}_s(s) = \left[\sum_{1}^{j} w_i \, e^{-\Delta t_i s} + \frac{1}{\beta} \left(\sum_{j+1}^{M} w_i \, e^{-\alpha \Delta t_i s} \right) \right. \left. \left(\sum_{j+1}^{M} w_i \, e^{-(1-\alpha) \, \Delta t_i s} \right) \right]$$

$$(\mu_1)_s = \sum_{j+1}^{M} w_i \, \Delta t_i + \sum_{1}^{j} w_i \, \Delta t_i = \sum_{1}^{M} w_i \, \Delta t_i = \mu_1$$

$$(\mu_2)_s = (\alpha^2 + (1-\alpha)^2) \left[\sum_{j+1}^{M} w_i \, (\Delta t_i)^2 - \frac{1}{\beta} \left(\sum_{j+1}^{M} w_i \, \Delta t_i \right)^2 \right] \qquad (41)$$

$$+ \frac{1}{\beta} \left(\sum_{j+1}^{M} w_i \, \Delta t_i \right)^2 + \sum_{1}^{j} w_i \, (\Delta t_i)^2$$

and

$$(\sigma_2)_s = (\mu_2)_s - (\mu_1)_s^2$$

Of course $\beta = 1$ gives the lowest value of the variance. In this case (j=1):

$$(\sigma_2)_s = (\alpha^2 + (1-\alpha)^2) \left(\sum_1^M w_i \, (\Delta t_i)^2 - \left(\sum_1^M w_i \, \Delta t_i\right)^2\right)$$

i.e. same as two mixing steps.

Furthermore, given β, $\alpha = 1/2$ again minimizes $(\sigma_2)_s$.

Finally, we will give a specific example. Assume that the flow is governed by the cubic law:

$$Q(\delta) = k_1 \, \ell \, \delta^3 \tag{42}$$

and:

$$\Delta t(\delta) = x/(k_1 \delta^2) \tag{43}$$

where ℓ is the fissure length perpendicular to the flow direction, x is the distance in the flow direction and k_1 is a constant.

For our "fundamental" unit (Figure 2a), using equation (32), we obtain:

$$\mu_n = \frac{k_1^{1-n} \, \ell x^n}{\bar{Q}} \int_0^\infty f(\delta) \, \delta^{3-2n} \, d\delta \tag{44}$$

and since $\mu_o = 1.0$ (or directly):

$$\bar{Q} = k_1 \, \ell \int_0^\infty f(\delta) \, \delta^3 \, d\delta \tag{45}$$

Snow (1970) studied the fissure frequencies $f(\delta)$ for various consolidated rocks including granites. He found the distribution to be log-normal.

$$f(\delta) = \frac{1}{\sigma_\ell \sqrt{2\pi}} \cdot \frac{1}{\delta} \exp \left[-1/2 \left(\frac{\ell n \, \delta - \mu_\ell}{\sigma_\ell} \right)^2 \right] \tag{46}$$

The distribution has the expected value:

$$E = e^{\mu_\ell + 0.5\sigma_\ell^2} \tag{47}$$

Substituting for $f(\delta)$ in equation (44) we obtain:

$$\mu_n = \frac{k_1^{1-n} \, \ell \, x^n}{\bar{Q} \, \sigma_\ell \sqrt{2\pi}} \int_0^\infty \delta^{2(1-n)} \exp \left| -1/2 \left(\frac{\ell n \delta - \mu_\ell}{\sigma_\ell} \right)^2 \right| d\delta \tag{48}$$

Making the substitution $y = \ell n\ \delta$ and using:

$$\int_{-\infty}^{\infty} \exp\ (-p^2x^2 \pm qx)\ dx = \exp\ (\frac{q^2}{4p^2})\ \frac{\sqrt{\pi}}{p}\ ,\quad p > 0$$

(Gradshteyn and Ryzhik, 1980, 3.323) together with equation (47) yields:

$$\mu_n = \frac{k_1^{1-n}\ \ell x^n}{\bar{Q}}\ E^{(3-2n)}\ e^{(3-2n)(1-n)\sigma_\ell^2} \tag{49}$$

and

$$\bar{Q} = k_1\ \ell\ E^3\ e^{3\sigma_\ell^2} \tag{50}$$

Combining (49) and (50) gives:

$$\mu_n = (\frac{x}{k_1})^n\ \frac{1}{E^{2n}}\ e^{n(2n-5)\sigma_\ell^2} \tag{51}$$

In particular:

$$\mu_1 = \frac{x}{k_1}\ \frac{1}{E^2}\ e^{-3\sigma_\ell^2}$$

and using equations (10) we obtain the central moments:

$$\mu_2' = \left(\frac{x}{k_1}\right)^2 \frac{1}{E^4} \left(e^{-2\sigma_\ell^2} - e^{-6\sigma_\ell^2}\right)$$

$$\mu_3' = \left(\frac{x}{k_1}\right)^3 \frac{1}{E^6} \left(e^{3\sigma_\ell^2} - 3e^{-5\sigma_\ell^2} + 2e^{-9\sigma_\ell^2}\right)$$

$$\mu_4' = \left(\frac{x}{k_1}\right)^4 \frac{1}{E^8} \left(e^{12\sigma_\ell^2} - 4 + 6e^{-8\sigma_\ell^2} - 3e^{-12\sigma_\ell^2}\right)$$

It is easy to show that $\mu_3' \geq 0$. Accordingly, the system response is skewed to the right, i.e. it has a tail with increasing time. We are now ready to derive:

$$\left(\frac{\sigma}{t}\right)^2 = e^{4\sigma_\ell^2} - 1$$

$$\gamma_1 = \frac{e^{3\sigma_\ell^2} - 3e^{-5\sigma_\ell^2} + 2e^{-9\sigma_\ell^2}}{\left(e^{-2\sigma_\ell^2} - e^{-6\sigma_\ell^2}\right)^{1.5}}$$

$$\gamma_2 = \frac{e^{12\sigma_\ell^2} - 4 + 6e^{-8\sigma_\ell^2} - 3e^{-12\sigma_\ell^2}}{\left(e^{-2\sigma_\ell^2} - e^{-6\sigma_\ell^2}\right)^2} - 3$$

As expected these quantities are dependent on σ_ℓ only. They are all very sensitive to σ_ℓ^2 and thereby to the fracture width distribution. In Figure 3, $(\frac{\sigma}{\bar{t}})^2$, γ_1 and γ_2 are plotted against σ_ℓ for $0 < \sigma_\ell < 0.5$. Note the very rapid increase, expecially for the coefficient of kurtosis, at higher values of σ_ℓ. Snow (1970) found σ_ℓ values between 0.057 and 0.394 with a mean 0.22. Values of $(\sigma/\bar{t})^2$, γ_1 and γ_2 for these specific σ_ℓ-values are given in Table 1.

If there was no intermediate mixing we would get an axial dispersion coefficient which increases linearly with distance according to equation (31), the slope being proportional to $(\sigma/\bar{t})^2$. Using the values in Table 1 yields $D_L/\bar{U}$ values between 0.0065x and 0.43x. Looking at the values for γ_1 and γ_2 we see that there is a considerable departure from a symmetric response, except at very low values of σ_ℓ (when the fracture aperture distribution is narrow).

We now turn to the situation with N mixing steps in series as depicted in Figure 2b. As discussed before, the equivalent dispersion coefficient will now attain a constant value determined by the spread in one mixing step. However, the system response may be far from Gaussian (as predicted by the diffusion-dispersion model) if the number of steps are not large enough. To obtain a criterion for when the distribution is approximately Gaussian we use equations (36)-(37) requiring γ_1 and γ_2 to be less than 0.5. The results are given in Table 1. It is seen that the number of steps is reasonable ($N < 10$) up

to the mean value of σ_ℓ but then rapidly increases. It is conceived that for higher values of σ_ℓ the diffusion-dispersion model will not be adequate to describe the dispersal behavior in fissured rock even at considerable transport distances.

σ_ℓ	$(\frac{\sigma}{\bar{t}})^2$	γ_1	γ_2	N from $(\gamma_1)_s<0.5$	N from $(\gamma_2)_s<0.5$
0.057	0.013	0.34	0.21	1	1
0.22	0.21	1.49	4.16	9	9
0.394	0.86	3.58	29.26	52	59

Table 1. Characteristic response parameters $(\sigma/\bar{t})^2$, γ_1 and γ_2 for the system depicted in Figure 2a assuming cubic law and log-normal fracture width distribution. Values of σ_ℓ are extreme values and mean value as found by Snow (1970). The last two columns give the minimum number of mixing-steps, as depicted in Figure 2b, required to obtain an approximately Gaussian (diffusion-dispersion like) response.

DISCUSSION AND CONCLUSIONS

In the preceding sections it has been demonstrated that the RTD-theory should be a powerful tool for gaining insight into the dispersal behavior of fracture networks. From a set of simple relations at least the first four statistical moments for the system response are easily obtained even for complicated networks. In particular an equivalent dispersion coefficient may be calculated from the second central moment (variance). From the examples it is seen that the effect of channeling generally decreases in systems with many mixing steps where the fluid particles lose their identity.

It is apparent from this discussion that Laplace domain solutions for the composite density function can be found for networks of large complexity, provided always that the subsystems remain statistically independent. Time domain solutions, however, may be difficult to obtain. Numerical solutions for f(t) based on inverse Laplace transformation may be ill-conditioned and thus computationally difficult. Computer simulation (e.g. Monte Carlo techniques) is a useful option in such circumstances.

The analysis performed here may be extended to more complicated systems. For example, non-zero volume of the mixing boxes can be taken into account (Appendix). The techniques described so far have been for systems having only a single inlet and a single outlet. Methods for treating systems having many connections with the environment are discussed by Nauman and Buffham (1983). Furthermore, the tools devel-

oped may, with little alteration, be used for layered media consisting of parallel (non-interacting or interacting) zones of different hydraulic conductivities causing a distribution in flow and retention times.

The theoretical analysis show that distribution of flow and retention times in the channels and their degree of connectivity have a strong impact on transport of a dissolved species in fractured rock. Unfortunately, such data are largely not available. However, we feel that the growing experimental evidence on channeling in fissured rock should warrant further research in this direction.

APPENDIX: Transfer function for mixing box with non-zero volume

Consider a well mixed box with volume V and flow rate Q. For a Dirac-pulse inlet condition the differential mass balance is:

$$V \frac{dC}{dt} = Q \left[\delta_D(t) - C\right] \tag{A1}$$

with:

$$C(0) = 0 \tag{A2}$$

From this it is easy to derive the transfer function, its inverse and the moments:

$$\tilde{f}(s) = \frac{1}{\tau} \frac{1}{s + \frac{1}{\tau}}$$

$$f(t) = \frac{1}{\tau} e^{-\frac{t}{\tau}} \tag{A3}$$

$$\mu_n = n!\ \tau^n$$

$$\kappa_n = (n-1)!\ \tau^n$$

where $\tau = V/Q$ is the mean residence time.

NOTATION

C	concentration in water	M/L^3
C_{in}	inlet concentration	M/L^3
C_{out}	outlet concentration	M/L^3
D_L	dispersion coefficient	L^2/T
E	expected value of log-normal fracture width distribution	L
$F(\delta_i)$	fraction of total numbers of fractures having a width δ_i ($\sim f(\delta)\, d\delta$)	
$f(\delta)$	fracture size distribution	L^{-1}
$f(t)$	density function for residence times	T^{-1}
$\tilde{f}(s)$	Laplace transform of $f(t)$	
H	Heaviside's step function	
k_1	constant	$L^{-1}\, T^{-1}$
ℓ	fissure length perpendicular to flow direction	L
M	number of subsystems in parallel	
N	number of subsystems in series	
$Q(\delta_i)$	flow rate in fractures having width δ_i	L^3/T
$\bar{Q}$	mean flow rate	L^3/T
s	Laplace transform parameter	T^{-1}
t	time	T
$\bar{t}$	mean residence time	T
Δt_i	residence time in a fracture of width δ_i	T
$U(\delta_i)$	velocity in fracture	L/T
$\bar{U}$	mean velocity	L/T
w_i	fraction of particle flow	
x	distance in flow direction	L

Greek symbols

α	relative position of intermediate mixing step (Figure 2c)	
β	fraction of total flow going through intermediate mixing step (Figure 2d)	
γ_1	coefficient of skewness	
γ_2	coefficient of kurtosis	
δ_D	Dirac delta function	
δ_i, δ	fissure width	L
κ_n	cumulant of order n	T^n
μ_ℓ	parameter in log-normal fracture width distribution	ℓn L
μ_n	moment about origin of order n	T^n
μ_n'	moment about mean of order n	T^n
σ^2	variance of residence times	T^2
σ_ℓ	"standard deviation" in log-normal fracture width distribution	

Subscript

i	parameter for channel of width δ_i
s	parameter for composite system

ACKNOWLEDGEMENT

This work was supported by the Swedish Nuclear Fuel Supply Company (SKB).

REFERENCES

Abelin, H., J. Gidlund, L. Moreno and I. Neretnieks: Migration in a single fracture in granitic rock, Scientific Basis for Nuclear Waste Management VII, Boston 1983. Proceedings North-Holland 26, 239-246, 1984.

Danckwerts, P.V.: Continuous flow systems: Distribution of residence times, Chem. Engng. Sci. 2, 1-13, 1953.

Eadie, W.T., D. Drijard, F.E. James, M. Roos and B. Sadoulet: Statistical Methods in Experimental Physics, North-Holland 1971.

Gradshteyn, I.S. and I.M. Ryzhik: Tables of Integrals, Series and Products. Academic Press, corrected and enlarged edition 1980.

KBS - Nuclear Fuel Safety Project, Final storage of spent nuclear fuel, KBS-3, Technical report, Stockholm 1983.

Levenspiel, O.: Chemical Reaction Engineering, 2nd ed., Wiley, 1972.

Levenspiel, O. and T.J. Fitzgerald: A warning on the misuse of the dispersion model, Chem. Engng. Sci. 38, 489-491, 1983.

Nauman, E.B. and B.A. Buffham: Mixing in Continuous Flow Systems, Wiley, 1983.

Neretnieks, I.: A note on fracture flow dispersion mechanisms in the ground, Water. Resour. Res. 19, 364-370, 1983.

Rasmuson, A. and I. Neretnieks: Migration of radionuclides in fissured rock: The influence of micropore diffusion and longitudinal dispersion, J. Geophys. Res. 86, 3749-3758, 1981.

Snow, D.T.: The frequency and apertures of fractures in rock. Int. J. Rock Mech. Min. Sci. 7, 23-40, 1970.

Sundaresan, S., N.R. Amundson and R. Aris: Observations on fixed-bed dispersion models: The role of the interstitial fluid, AIChE J. 26, 529-536, 1980.

Zwietering, T.N.: The degree of mixing in continuous flow systems, Chem. Engng. Sci. 11, 1-15, 1959.

FIGURES

Figure 1 Rules for summing flow streams

(a) Flow division point

(b) Flow combination point

Figure 2 Fracture networks treated

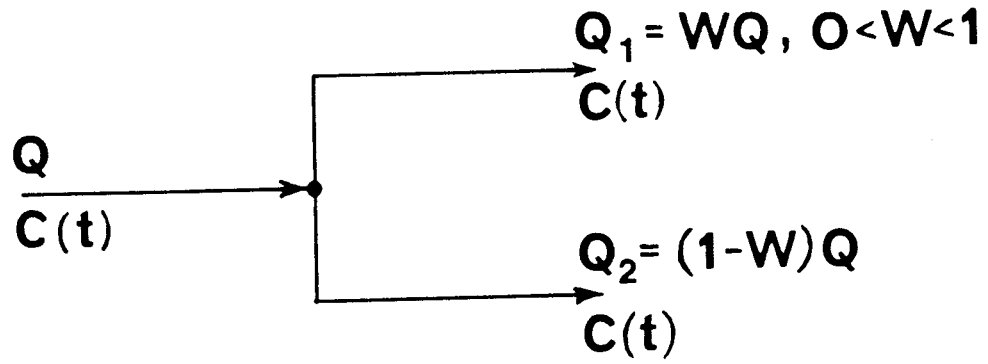
(a) "Basic" unit. Set of parallel fractures with a common inlet and outlet. The fracture widths $F(\delta_i)$, flow in each fracture $Q(\delta_i)$ and retention times $\Delta t(\delta_i)$ are arbitrarily distributed.

(b) Composite system consisting of N units as in (a) in series.

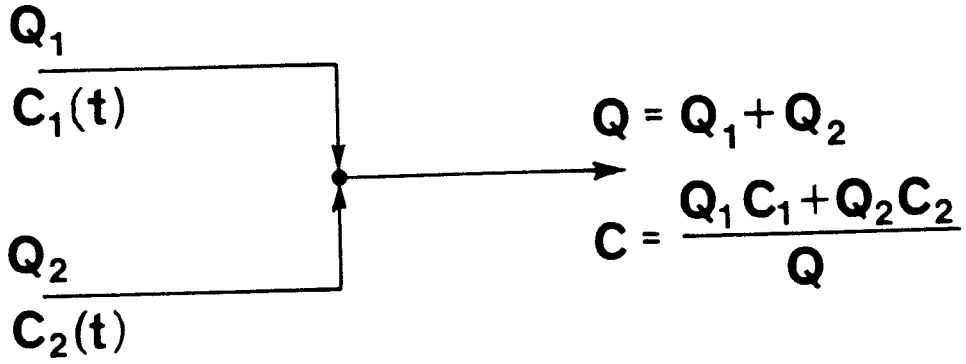
(c) Effect of location (α) of intermediate mixing step.

(d) Effect of partial mixing step at arbitrary (α) intermediate location. A fraction ($1-\beta$) of the total flow, Q, is flowing through fractures with sizes 1 to j and fraction β through channels > j.

Figure 3 The quantities $(\sigma/\bar{t})^2$, γ_1 and γ_2 for the system depicted in Figure 2a as a function of σ_ℓ. Flow distribution according to cubic law and log-normal fracture width distribution.

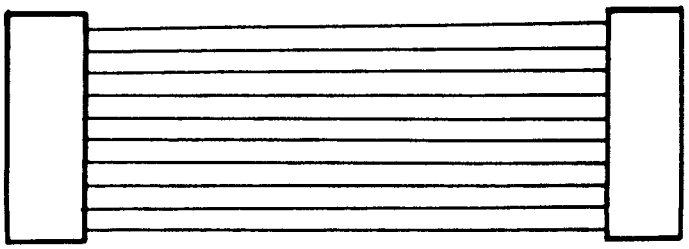


(a)

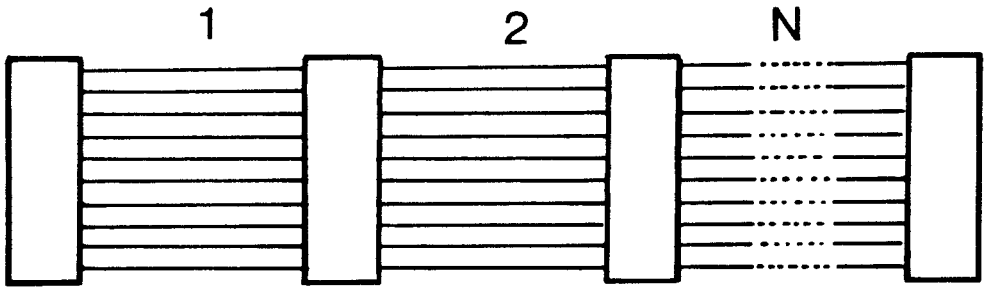


(b)

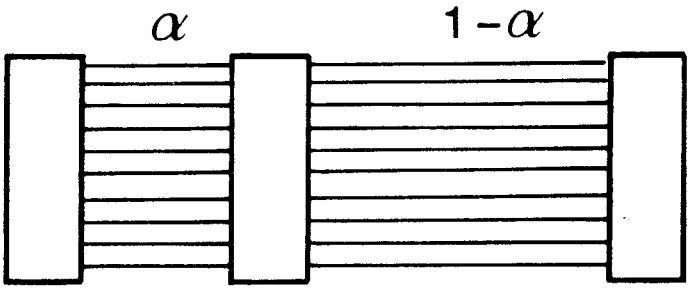
Figure 1



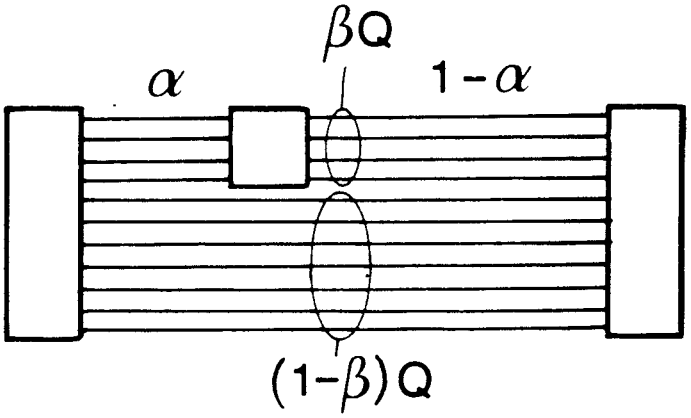
(a)



(b)



(c)



(d)

Figure 2

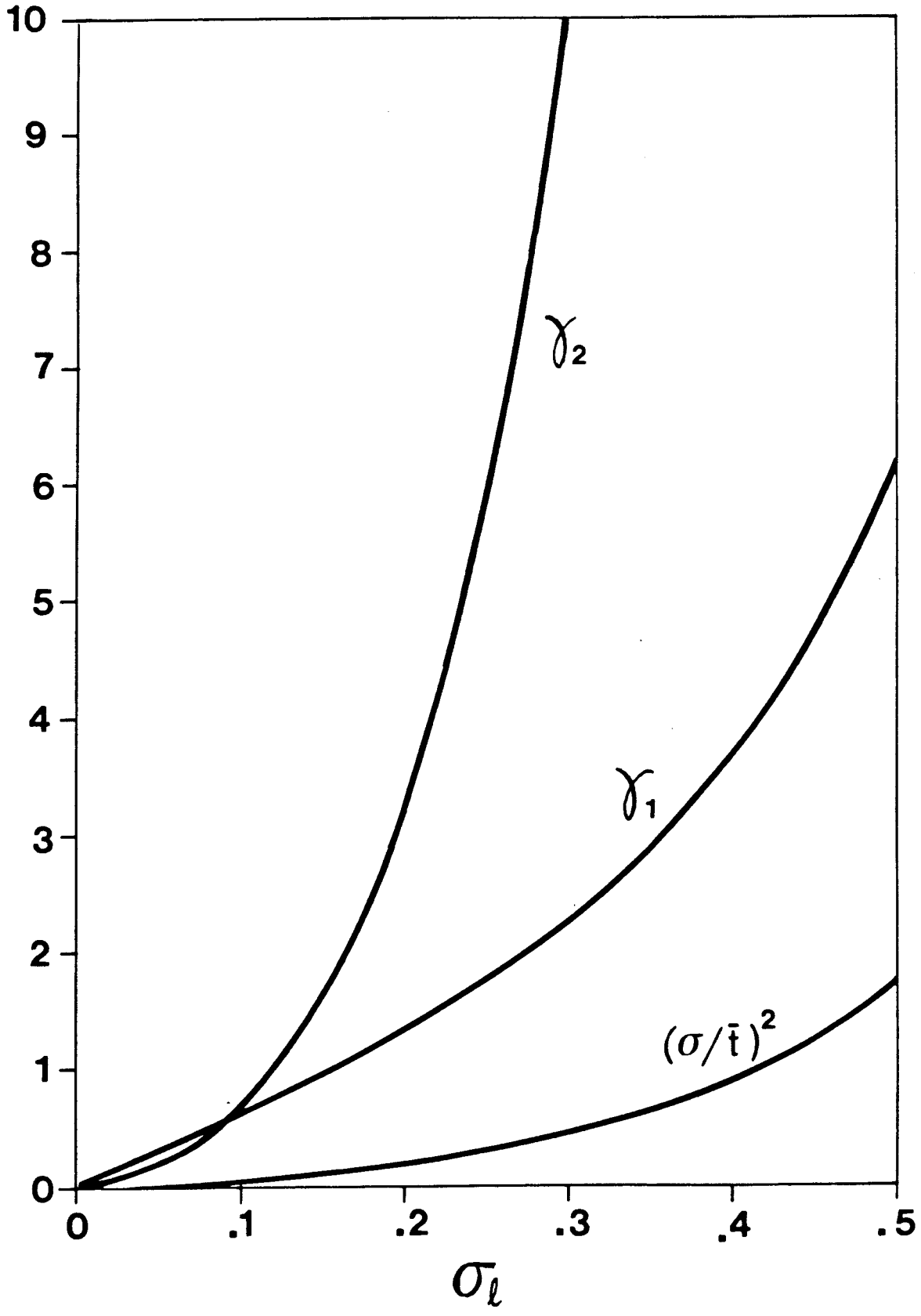


Figure 3

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.

1980
TR 80–26
The KBS Annual Report 1980.
KBS Technical Reports 80-01 – 80-25.
Summaries. Stockholm, March 1981.

1981
TR 81–17
The KBS Annual Report 1981.
KBS Technical Reports 81-01 – 81-16.
Summaries. Stockholm, April 1982.

1982
TR 82–28
The KBS Annual Report 1982.
KBS Technical Reports 82-01 – 82-27.
Summaries. Stockholm, July 1983.

1983
TR 83–77
The KBS Annual Report 1983.
KBS Technical Reports 83-01 – 83-76
Summaries. Stockholm, June 1984.

1984
TR 85–01
Annual Research and Development Report 1984
Including Summaries of Technical Reports Issued during 1984. (Technical Reports 84-01– 84-19)
Stockholm June 1985.

1985
TR 85–01
Annual Research and Development Report 1984
Including Summaries of Technical Reports Issued during 1984.
Stockholm June 1985.

TR 85–02
The Taavinunnanen gabbro massif. A compilation of results from geological, geophysical and hydrogeological investigations.
Bengt Gentzschein
Eva-Lena Tullborg
Swedish Geological Company
Uppsala, January 1985

TR 85–03
Porosities and diffusivities of some non-sorbing species in crystalline rocks.
Kristina Skagius
Ivars Neretnieks
The Royal Institute of Technology
Department of Chemical Engineering
Stockholm, 1985-02-07

TR 85–04
The chemical coherence of natural spent fuel at the Oklo nuclear reactors.
David B. Curtis
New Mexico, USA, March 1985

TR 85–05
Diffusivity measurements and electrical resistivity measurements in rock samples under mechanical stress.
Kristina Skagius
Ivars Neretnieks
The Royal Institute of Technology
Department of Chemical Engineering
Stockholm, 1985-04-15

TR 85-06
Mechanical properties of granitic rocks from Gideå, Sweden
Christer Ljunggren
Ove Stephansson
Ove Alm
Hossein Hakami
Ulf Mattila
Div of Rock Mechanics
University of Luleå
Luleå, Sweden, October 1985

TR 85-07
Complex forming properties of natural occurring fulvic acids
Part 1. Complexes with cadmium, copper and calcium
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
Concentration and distribution of natural radionuclides at Klipperåsen and Bjulebo, Sweden
Björn Sundblad, Ove Landström, Rune Axelsson
Studsvik Energiteknik AB, Nyköping, Sweden

TR 85-10
Chemical interactions between the bentonite and the natural solutions from the granite near a repository for spent nuclear fuel
Bertrand Fritz and Marie Kam
Université Louis Pasteur de Strasbourg, Institut de Géologie, France
July 1985

TR 85-11
Hydrochemical investigations in crystalline bedrock in relation to existing hydraulic conditions: experience from the SKB test-sites in Sweden
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