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A note on dispersion mechanisms in the ground

Ivars Neretnieks

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A NOTE ON DISPERSION MECHANISMS IN THE GROUND

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SUMMARY

Two mechanisms for the spreading of a tracer pulse are discussed. Stratified flow and diffusion in the rock matrix are normally not accounted for when the hydrodynamic dispersivity is evaluated from tracer tests in the ground. It is shown that where there is stratified flow, the spreading of a tracer pulse cannot be described by the Fickian diffusion - dispersion approach. If a dispersion coefficient were evaluated from such an experiment, the dispersion coefficient would grow proportionally to the observation distance.

When a tracer flowing with the water in the channels of a geologic medium can diffuse into the porous matrix of the solid, a tracer pulse will spread. The spreading due to this mechanism cannot be described by Fickian dispersion. In a special case when the time for matrix penetration is long, the observed tracer pulse will have an infinitely long tail. If the conventional moment method is used to determine a dispersion coefficient in such cases, the results will depend on the detection limit of the tracer to a very large extent.

Background

By dispersion in a very broad sense we mean the spreading of a species carried by a fluid as the fluid moves along a flow path. Figure 1 gives an example of such spreading when a tracer is introduced at one point.

There are many mechanisms contributing to such spreading:

- Molecular diffusion in the liquid
- Velocity variations in the fluid in a channel
- Velocity variations between channels in a porous medium
- Chemical or physical interactions with the solid material

Molecular diffusion does not contribute much to the spreading of the front when large distances are considered. On the contrary it will diminish dispersion arising from velocity variations within a channel as the concentration difference over the channel width will be decreased by diffusion. In the case of flow in low permeability fissured rock the concentrations over the fissure width for all practical purposes can be considered constant.

Velocity variations between channels is a very important dispersion mechanism. Bear (1969) gives a comprehensive treatment on hydrodynamic dispersion theories.

The most advanced models treat the spreading process by modelling more or less randomly oriented pores combined with some assumptions on how velocities in the channels vary as well as how distribution at channel divisions and mixing at channel intersections occur. An early but fairly advanced such treatment is found in de Josselin de Jongs paper (1958).

The common basis for practically all these treatments is that the spreading is described by one parameter - the standard deviation σ_x (or variance σ_x^2) of a pulse as it spreads with distance. Figure 2 shows the standard deviation of a pulse which is spreading as it moves along a flow path.

If the spreading were a random process such as molecular diffusion, a dispersion coefficient D_L analogous to the diffusion coefficient could be determined from $D_L = \frac{\sigma_x^2}{2\bar{t}}$. In most treatments of the dispersion process it is more or less implicitly assumed that this is the case. For porous media with fairly uniform particle size this has been verified experimentally by many independent investigators.

For beds of uniform particle size very good agreement between experimental results and model predictions are obtained (Bear p. 168) if the distance travelled is considerably longer than the particle size.

The dispersion coefficient is proportional to the velocity and the particle size; $D_L \propto U_f d_p$. This also implies that the variance is proportional to the distance

$$\sigma_x^2 \propto x$$

In some investigations however, it has been noted that if the beds are not carefully packed the dispersion may increase considerably. The explanation for this is usually summarized in the word "channeling" or "uneven distribution". Recently Schwarz (1977) by computer simulation has shown that the uneven distribution of resistances in a porous medium may not lead to a variance which increases proportionally to the distance travelled. Neretnieks (1977) showed that in a medium where severe channelling occurs - parallel unconnected channels with velocity differences between channels - the standard deviation σ_x is proportional to the distance travelled

$$\sigma_x \propto x$$

instead of $\sigma_x^2 \propto x$ as in the diffusion-dispersion case above.

Recently Matheron and Marsily (1980) arrived at the same conclusion and also conclude that the usual "convection diffusion equation" cannot in general be applied even for large distances.

For flow in a porous medium the diffusion-dispersion, where $\sigma_x^2 \propto x$, will give the lower bound on the spreading of the front. The stratified flow case may in some cases give an upper bound on the spreading of a concentration pulse. To the authors knowledge all field data on dispersion have so far been more or less implicitly interpreted as being caused by diffusion-dispersion. Experimental resluts are interpreted by calculating the dispersion coefficient D_L.

Lallemand-Barrès and Peaudecerf(1978) compiled a lot of field data. Their figure 2 shows D_L/U_f versus the distance between injection point and observation point. Although the spread in data is large, there is a definite increase in D_L/U_f with distance which ranges from 3 m to 5 000 m. The swarm of points may fairly be approximated by D_L/U_f = const · x. With const ≃ ≃ 0.1, 90 % of the points lie within the bounds $\frac{U_f x}{D_L} = 1\text{-}30$.
The hypothesis that the dimensionless quantity $U_f x/D_L$, which is commonly called the Peclet number, is constant is much better than the hypothesis that D_L/U_f is constant. The first spans over 1.5 orders of magnitude whereas the second spans over more than 2.5 orders of magnitude. Field data thus do not indicate that D_L/U_f is constant. The spread for both models is so great that the proper model cannot be identified from these data. As, however, the implications of using the wrong mechanism when using a model for extrapolation to large distances may have very grave consequences in some applications, it is necessary to investigate the stratified flow model also. This

is the more important because practically all effort over the last decades has gone into refining the diffusion-dispersion model and very little effort has gone towards a consequent study of the other extreme alternative.

Later a stratified flow model will be presented and the consequences of this as compared to the use of the diffusion-dispersion model for predicting the migration of radionuclides in a fissured bedrock will be discussed.

A mechanism of "dispersion" which does not seem to be treated in the hydraulic literature is the effect of interaction with the solid material. Here only one such aspect will be discussed - that of diffusion of the species into the rock matrix. In the chemical engineering literature Kučera (1965), (Perry 10-23) this effect is not treated as dispersion but modelled independently and thus separated from the hydrodynamic dispersion. For many cases involving diffusion into the solids, the shape of the breakthrough front is more determined by this mechanism than by hydrodynamic dispersion. It has been shown (Neretnieks 1980) that these effects may have a considerable influence on the breakthrough curve for flow in fissured granitic bedrock.

Stratified flow

An attemt to quantify the variance and dispersion for the case of flow in a set of parallel fissures is done below. It is based on the assumption that the fissures act as independent channels with no mixing occurring between them. At the inlet end of the channels a tracer can be introduced. This is done simultaneuosly in all fissures. At some distance downstream the fluid from all channels is collected and mixed. The concentration in this point is measured over time, as some fissures carry the tracer faster than others, a narrow pulse at the inlet will have spread when observed at the outlet. The residence time distribution and its mean and variance can be determined from the observed concentration-time curve. If the variance of the tracer pulse at the inlet is known, the dispersion coefficient can be determined from (Levenspiel 1972)

$$\frac{\sigma^2_{t,out} - \sigma^2_{t,in}}{\bar{t}^2} = 2\,\frac{D_L}{\bar{U}\,x} \qquad (1)$$

Determination of the variance for a breakthrough curve from parallel fissure flow

The fissure width distribution is $f\,(\delta)$. In a fissure of width δ_i with laminar flow,the flow rate $Q(\delta_i)$ is proportional to the fissure width to the third-power

$$Q(\delta_i) = k_1 \delta_i^{\,3} l \qquad (2)$$

where l is the length of the fissure perpendicular to the flow. The velocity is proportional to the fissure width squared:

$$U_i = k_1 \delta_i^{\,2} \qquad (3)$$

The residence time in fissures with width δ_i over a given distance x is:

$$t_i = \frac{x}{k_1 \delta_i^2} \tag{4}$$

If a step with concentration C_o is introduced at the inlet end of the set of fissures, it will travel the distance x in time t_i in fissures with width δ_i. The fissures with residence times less than t will carry tracer. This is shown in Fig. 3.

The concentration obtained at the outlet end, at a time t when the effluent from all fissures is mixed is:

$$\frac{C(t)}{C_o} = \frac{\int_{\delta}^{\infty} f(\delta)\ Q(\delta)\ d\delta}{\int_{0}^{\infty} f(\delta)\ Q(\delta)\ d\delta} = \frac{Q_t}{\overline{Q}} \tag{5}$$

t is the residence time in fissure $\delta(t)$. The above expression says that the flow Q_t from the tracer carrying fissures with widths $\delta(t) \leq \delta < \infty$ is diluted by the total flow of water Q from all fissures.

The result for a Dirac concentration pulse at the inlet i.e $C_o\ dt = 1$ and $dt' \to 0$ can be obtained by differentiation of equation 5 with respect to time. It can also be derived directly as is shown in appendix 1.

$$\frac{C(t)}{C_o dt} = \frac{1}{2} k_1 \frac{f(\delta)\ Q(\delta)\ \delta^3}{x\ \overline{Q}} \tag{6}$$

where

$$\overline{Q} = \int_{0}^{\infty} f(\delta)\ Q(\delta)\ d\delta \tag{7}$$

The mean residence time for a response curve C(t) is obtained from

$$\overline{t} = \frac{1}{C_o dt} \int_{0}^{\infty} C(t)\ t\ dt \tag{8}$$

and the variance or second statistical central moment from

$$\sigma_t^2 = \frac{1}{C_o dt} \int_o^\infty C(t)\ (t-\bar{t})^2 dt \qquad (9)$$

By inserting equations 6,7,2 and 4 into 8 and 9 we obtain

$$\bar{t} = \frac{x}{\bar{Q}}\frac{1}{} \int_o^\infty f(\delta)\delta d\delta = \frac{x}{k_1} \frac{\int_o f(\delta)\delta d\delta}{\int_o^\infty f(\delta)\delta^3 d\delta} \qquad (10)$$

and

$$\frac{\sigma_t^2}{\bar{t}^2} = \frac{\int_o^\infty f(\delta)\delta^3 d\delta \cdot \int_o^\infty \frac{f(\delta)}{\delta} d\delta}{[\int_o^\infty f(\delta)\delta d\delta]^2} - 1 \qquad (11)$$

equation 11 shows that $\frac{\sigma_t^2}{\bar{t}^2}$ is independent of the distance. For the Dirac pulse at the inlet the variance is 0 and thus equation 1 directly gives

$$D_L = \frac{\sigma_t^2}{\bar{t}^2} \cdot \frac{1}{2}\,\bar{\bar{U}}\,x.$$

Thus $D_L \propto x$ for stratified flow.

Snow (1970) obtained the fissure frequencies $f(\delta)$ for various consolidated rocks including granites. Snow used data from water injection tests in boreholes and from direct measurements of fissure widths. He found the distribution to be log normal

$$f(\frac{\delta}{\mu}) = \frac{1}{A} \cdot e^{-\frac{1}{2}\left(\frac{\log\frac{\delta}{\mu}}{\sigma_1}\right)^2} \qquad (12)$$

The standard deviations σ_1 range from 0.057 to 0.394. The mean of σ_1 in Snow's investigation is 0.22. This will be the value used in the subsequent sample calculations. Fig. 4 shows the response to a Dirac pulse as determined by equation 6.

Using equation 12 we obtain $(\frac{\sigma_t}{\bar{t}})^2 = 1.82$ and $\frac{\sigma_t}{\bar{t}} = 1.35$

From equation 1 we obtain

$$\frac{D_L}{\bar{U}} = \frac{x}{2} \left(\frac{\sigma_t}{\bar{t}}\right)^2 \tag{13}$$

as $\sigma^2_{t,in} = 0$ for a Dirac pulse.

With the above value of the variance equation 13 predicts

$$\frac{D_L}{\bar{U}} = 0.91\,x.$$

The parallel fissure flow model thus predicts that the dispersion coefficient is proportional to the distance between the injection point and the observation point. It is also proportional to the velocity.

The recent compilation of dispersion coefficients obtained from field measurements by Lallemand-Barrès and Peaudecerf (1978) show this tendency. Although their data are very scattered the relation predicted above falls well within their datapoints.

Matrix diffusion

Another dispersion mechanism which also cannot be made to fit the conventional dispersion model is the spreading of the front due to physical or chemical interaction with the solid material. Kučera (1965) treats some cases of general interest. Only one special case of interaction will be treated here, namely the diffusion into the rock matrix of the fissure walls. This case has been treated recently by Neretnieks (1980) and is only summarized here.

When water which contains a tracer flows in a fissure, the tracer will migrate into the porous structure of the rock by diffusion. The water will thus be depleted of the tracer. For a case where the distance between the fissures is very large and where the tracer thus does not penetrate more than a fraction of the distance between fissures, the transport can be mathematically described by the following expressions.

Diffusion in the rock is given by:

$$\frac{\partial c_p}{\partial t} = D_a \frac{\partial^2 c_p}{\partial z^2} \qquad (14)$$

where $D_a = \frac{D_e}{K}$

For flow and sorption from the water in the fissure we have:

$$\frac{\partial c_f}{\partial t} + U_f \frac{\partial c_f}{\partial x} = \frac{2D_e}{\delta} \cdot \frac{\partial c_p}{\partial z}\Big|_{z=0} \qquad (15)$$

For a system which is initially free of tracer and where the tracer concentration suddenly is increased to C_o at the inlet of the fissure ($x = 0$), the initial and boundary conditions are:

IC	$C_p = C_f = 0$	$t = 0$, all x and z	(16)
BC1	$C_p = 0$	when $t > 0$ for $z \to \infty$	(17)
BC2	$C_f = C_o$	at $x = 0$ for $t > 0$	(18)

The solution is available in the literature (Carslaw & Jaeger 2nd ed. p. 396).

For the fluid in the fissure and for $t > \frac{x}{U_f}$ the following expression results:

$$\frac{C_f}{C_o} = \operatorname{erfc}\left(\frac{G}{\sqrt{t-t_w}}\right) \tag{19}$$

where $G = \frac{2D_e\ t_w}{\delta\sqrt{D_a}}$ and $t_w = \frac{x}{U_f}$

For a unit pulse at the inlet i.e $C_o\ dt = 1$ and $dt \to 0$, the response at the outlet is obtained by differentiation of equation 19 with respect to time

for $t > t_w$

$$\frac{C_f}{C_o dt} = \frac{\arg}{(t-t_w)\sqrt{\pi}} \cdot e^{-\arg^2} \tag{20}$$

$$\text{where } \arg = \frac{G}{\sqrt{t-t_w}} \tag{21}$$

The same result is of course obtained by using the Dirac pulse as boundary condition BC2 instead of equation 18 and solving equations 14 and 15.

The maximum for this function is at

$$t = t_w + 2/3\ G^2 \tag{22}$$

With the aid of equations 8 and 9 it could be attempted to find the mean residence time and variance of this residence time distribution. We find however that

$$\frac{C_f}{C_o dt} \propto \frac{1}{t^{3/2}} \quad \text{for } t \to \infty$$

and equations 8 and 9 thus are unbounded. This means that there is neither a mean residence time nor a variance if there is any diffusion into the porous walls and if the penetration depth is small compared to the distance to the next fissure. As most known rocks are more or less porous, this means that in priciple it is impossible to determine a dispersion coefficient by determining first and second moments of a response curve without first accounting for the matrix diffusion effect. The dispersion coefficients so far gathered in the literature may possibly have been obtained only because the integration of equations 8 and 9 were discontinued due to limited detection capability of the tracer at the tail of the pulse.

An example is used to demonstrate the importance of the detection limit. The case chosen is the following:
There is steady flow in a fracture where a tracer pulse is introduced at one point and the response is measured at another point 22 m downstream. The gradient over the fracture is 0.11 m/m, the rock matrix has an effective diffusivity $D_e = 10^{-12}$ m^2/s, an apparent diffusivity $D_a = 2 \cdot 10^{-10}$ m^2/s. and the water transport time is 10 hours. The D_e and D_a values are chosen to describe the diffusion of solved ions in the water in the pores in the rock matrix. There are no sorption effects and the rock porosity is 0.5 % which is a good value for a granite. Further details on diffusivities are given in Neretnieks (1980). For laminar flow of water in a parallel fissure at ambient temperature, the fissure width δ is 0.082 mm.

The species will diffuse into the rock matrix with a penetration depth of about 10 mm during a 10 h contact time. The condition that the tracer should penetrate only a fraction of the block size of the rock is well fullfilled for most crystalline rocks such as granites and gneisses where the distances between fissures usually is considerably more than 20 mm.

The response at the outlet is shown in figure 5. It has been calculated using equation 22. Two detection limits 1 % and 5 % are indicated by the dashed lines. The figure shows the long tail which gives an infinite mean residence time and variance. Table 1 shows the mean residence time $\bar{t}$, the relative standard deviation $\frac{\sigma_t}{\bar{t}}$, the dispersion coefficient D_L and evaluated Peclet number Pec for the detection limits 0.2, 1 and 5 %. It is clear that the detection limit will have a dominating influence on the results.

Even in this case when the peak is fairy narrow, the long tail will give a high dispersion coefficient although there is no hydrodynamic dispersion.

An increasing water transport time will quickly aggravate the problem. Table 2 shows the same case as in table 1 but with twice the residence time -20 h instead of 10 h. For 1 % detection level the evaluated Peclet is 8. This is well within the range of Peclet numbers found in the field as was described earlier.

Table 1

detection limit %	0	0.2	1	5
$\bar{t}$ s	∞	46800	42000	39200
$\frac{\sigma_t}{\bar{t}}$	∞	0.39	0.18	0.078
D_L m^2/s	∞	$7.9 \cdot 10^{-14}$	$1.84 \cdot 10^{-4}$	$3.32 \cdot 10^{-5}$
Pec	0	13	62	330

Table 2

detection limit %	0	1	5
$\bar{t}$ s	∞	120000	97700
$\frac{\sigma_t}{\bar{t}}$	∞	0.5	0.24
D_L m^2/s	∞	$5.06 \cdot 10^{-4}$	$1.31 \cdot 10^{-4}$
Pec	0	8.0	36

Discussion

The possibility of stratified flow in fissured rock may have important implications on the migration of radionuclides from a leaking repository for spent fuel. If field experiments are interpreted using the diffusion-dispersion model wich implies a constant dispersion coefficient , an extrapolation to large distances will show that the front becomes narrower if related to the mean distance travelled; $\sigma_x/x \propto \frac{1}{\sqrt{x}}$. One might finally be led to believe that there essentially is no dispersion over very large distances! For perfectly stratified flow the front will keep its form and $\frac{\sigma_x}{x}$ = const. This means that at a given fraction of the mean residence time, the same fraction of the tracer will have arrived. For a decaying radioactive tracer this may in some cases mean that the radionuclide which would have decayed to insignificance during the mean residence time, will not have had time to decay for the fraction which arrives earlier.

Dispersion due to diffusion into and out of the particles cannot be described by a dispersion coefficient D_L. The variance of a breakthrough front cannot in general be expressed in a simple way. In fact for the case where the particles into which the diffusion takes place are so large that the penetration depth is less than the particle size but large compared to the channel where flow takes place, the breakthrough curve has neither a mean residence time nor a variance. The use of conventional methods to determine the dispersion coefficient may give any result and is entirely dependent on the detection limit.

These effects have usually not been considered when tracer tests in the ground have been evaluated. For short contact times the diffusion is of little importance but already for contact times of days in a fissured and porous rock this effect may have a considerable influence on the widening of the front.

Conclusions

It is doubtful if the diffusion-dispersion description of tracer movement in fissured bedrock is applicable.

NOTATION

C	concentration in the liquid	mol/m^3
C_o	initial concentration in the liquid	mol/m^3
C_f	concentration in the liquid in a fissure	mol/m^3
C_p	concentration in the liquid in a pore	mol/m^3
d_p	particle diameter	m
D_a	apparent diffusivity $D_a = D_e/K$	m^2/s
D_e	effective diffusivity	m^2/s
D_L	dispersion coefficient	m^2/s
K	volume equilibrium constant	m^3/m^3
l	fissure length perpendicular to flow direction	m
Pec	Peclet number $\frac{\overline{U} \cdot x}{D_L}$	-
Q	flow rate	m^3/s
$\overline{Q}$	mean flow rate	m^3/s
Q_t	flow rate carrying tracer	m^3/s
t	time	s
$\bar{t}$	mean time	s
t_w	water residence time	s
dt	time for tracer injection $(dt \to 0)$	s
$\overline{U}$	mean velocity	m/s
U_f	velocity in a fissure	m/s
x	distance in flow direction	m
z	distance into rock matrix	m
δ	fissure width	m
σ_l	standard deviation in the logarithm of fissure widths	-
σ_t	standard deviation in the residence time distribution	s
σ_x	standard deviation in the spreading of a tracer pulse	m

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Derivation of the response to a Dirac pulse

During a short time dt a tracer with concentration C_o is injected at the inlet end of the set of parallel fissures. $C_o\, dt = 1$.

At the outlet end at distance x, it will take a time t for the tracer to arrive. The measurement or collecting time is dt during which time fissures with widths between δ-$d\delta$ and δ will have carried the tracer. The relation between $d\delta$ and dt is obtained by differentiating equation 4.

$$d\delta = - \frac{k_1 \delta^3}{2x} dt$$

The flow which carries tracer during this time is δ

$$Q_t = \int_{\delta - d\delta}^{\delta} f(\delta)\cdot Q(\delta) d\delta = \lim_{dt \to 0} f(\delta)\; Q(\delta)\; \frac{k_1 \delta^3}{2x} dt$$

The amount of tracer carried is $Q_t \cdot C_o$ and this is diluted in the total flow $\overline{Q}$. The observed concentration thus is

$$C(t) = \frac{Q_t C_o}{\overline{Q}} = C_o dt \cdot \frac{1}{2} k_1 \frac{f(\delta)\; Q(\delta)\; \delta^3}{x\; \overline{Q}}$$

Which is the same result as equation 6.

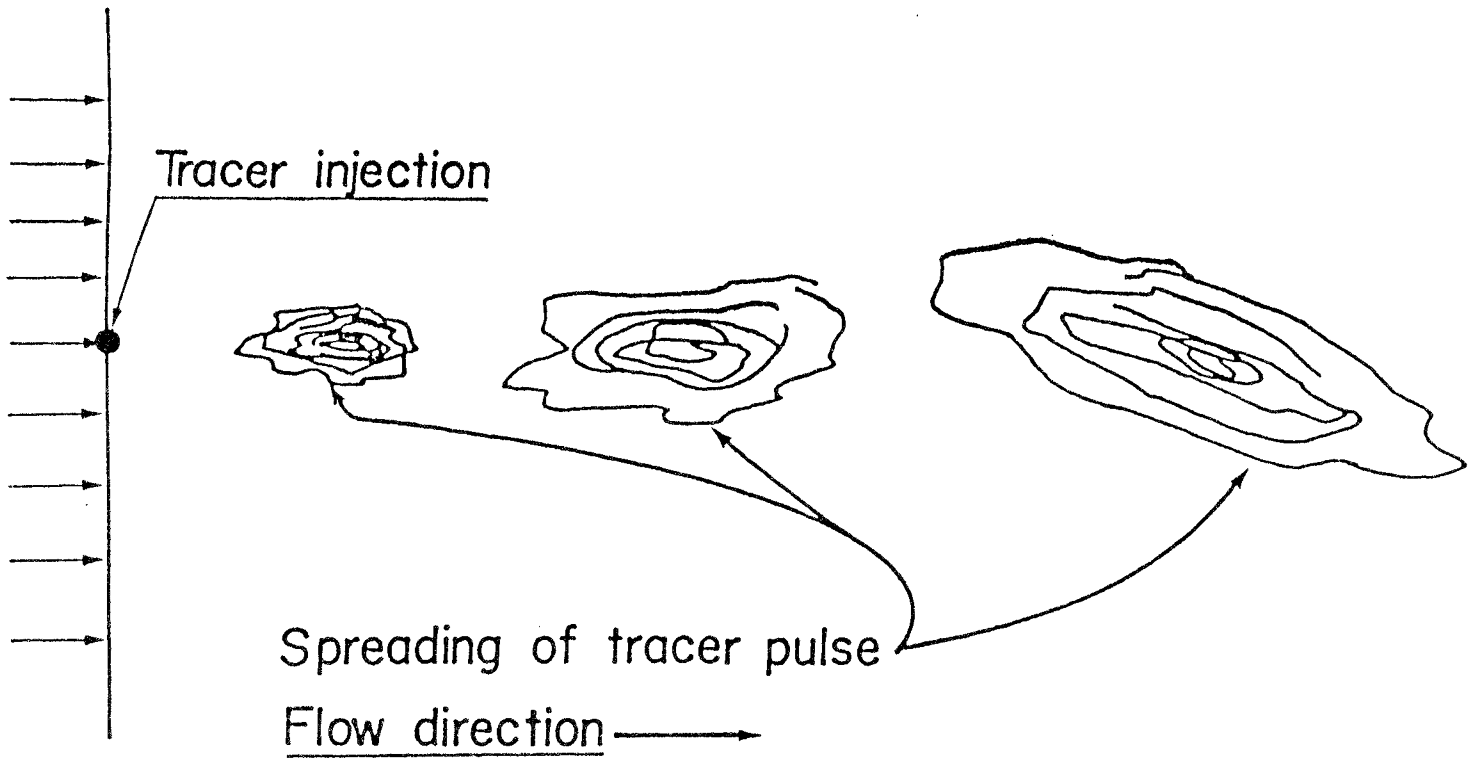

Figure 1 The spreading of a tracer injected at a point, as it follows the fluid.

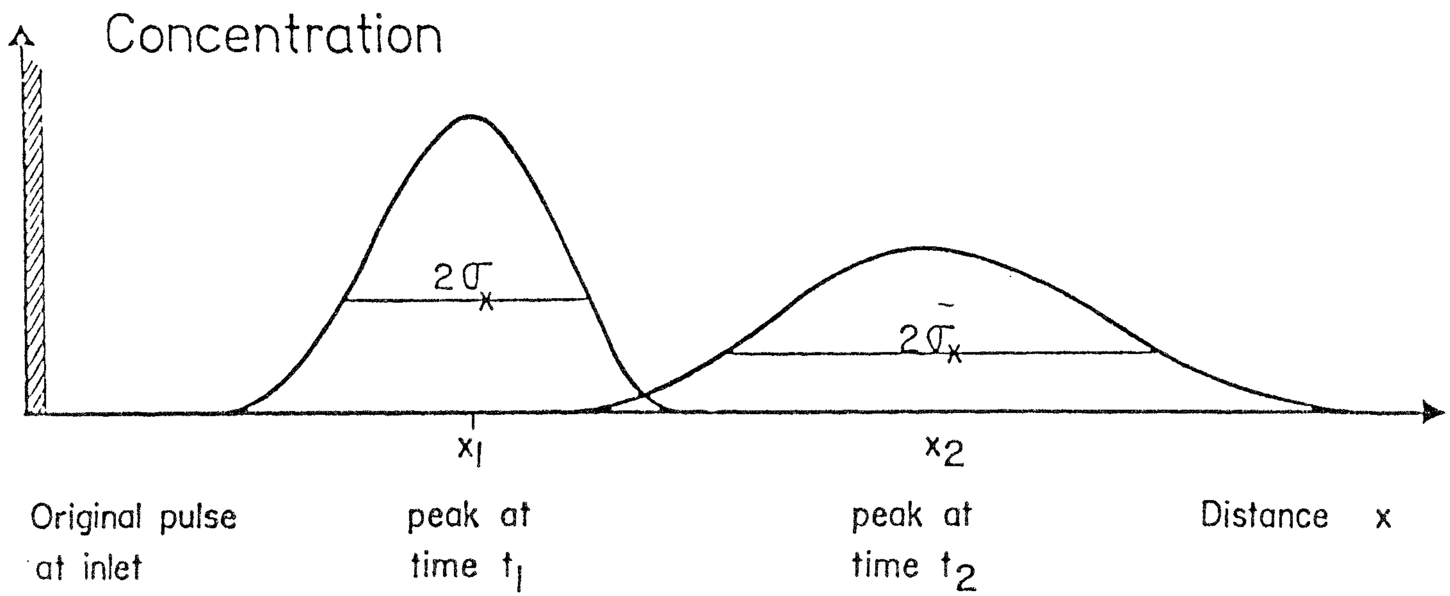

Figure 2 The concentration profile and the standard deviation of a tracer at different times.

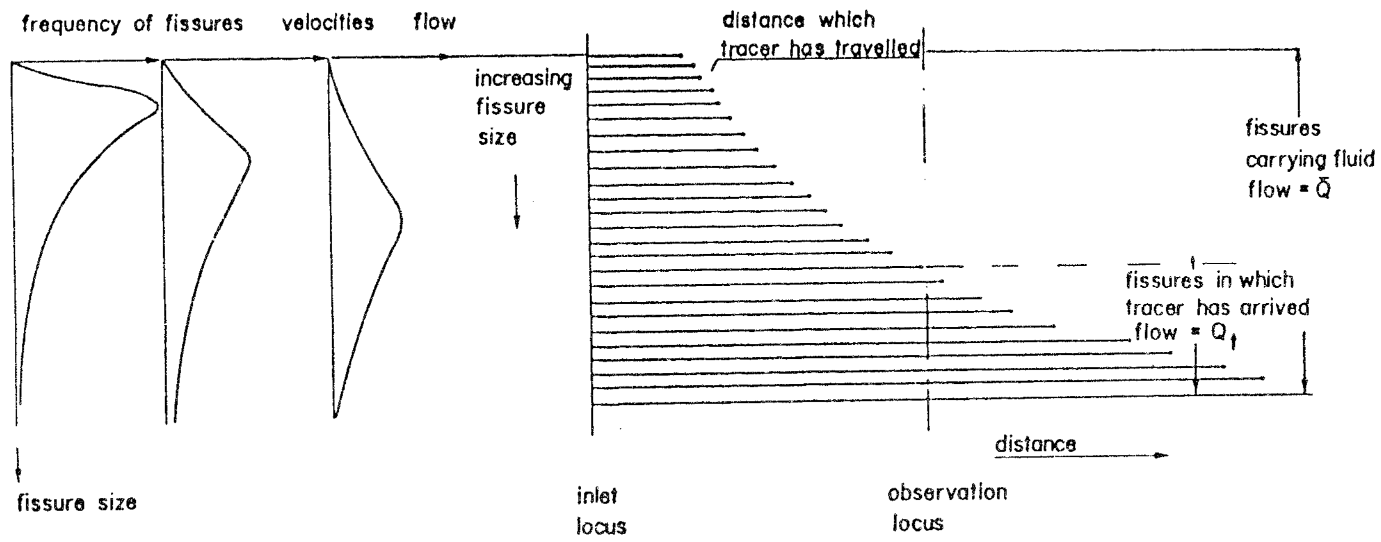

Figure 3 The locus of tracer carrying fluid in a medium with parallel fissures of different size.

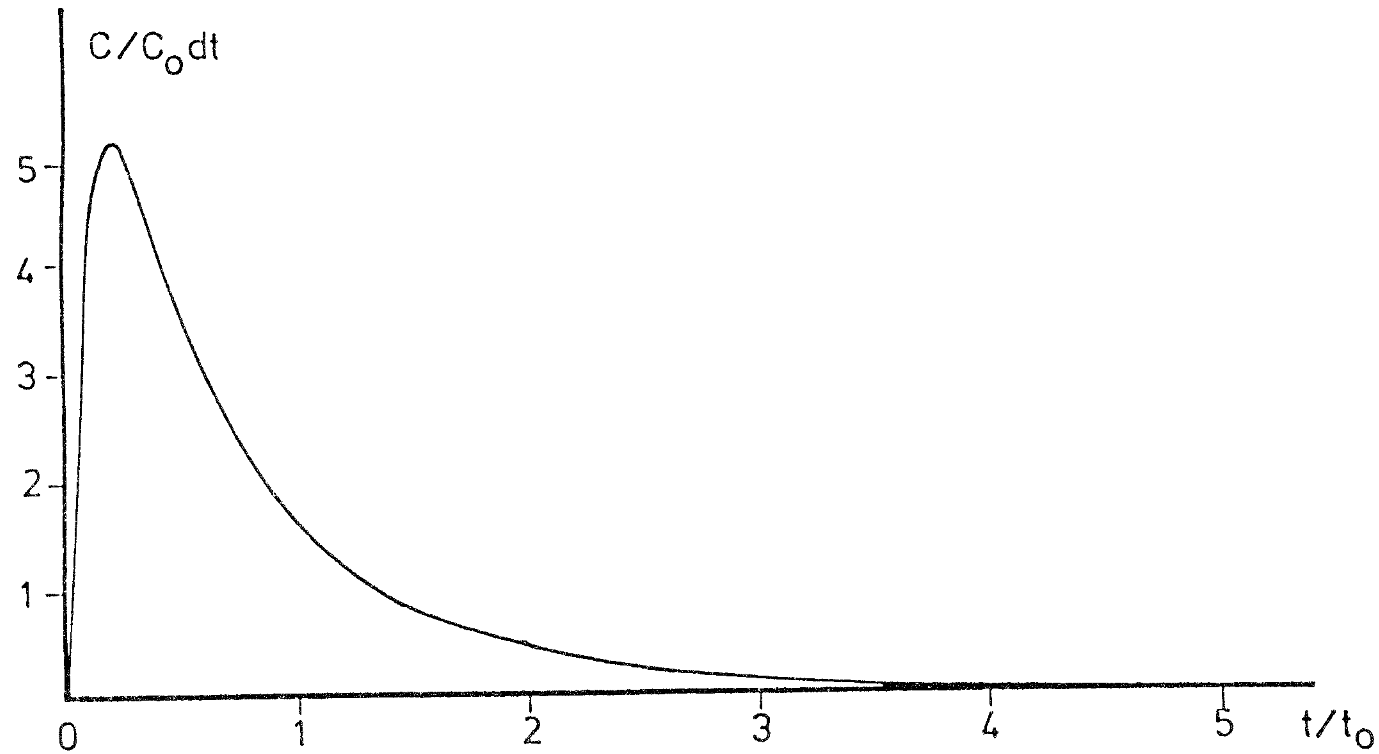

Figure 4 Concentration at the outlet of a medium with parallel fissures which has been injected with a tracer pulse.

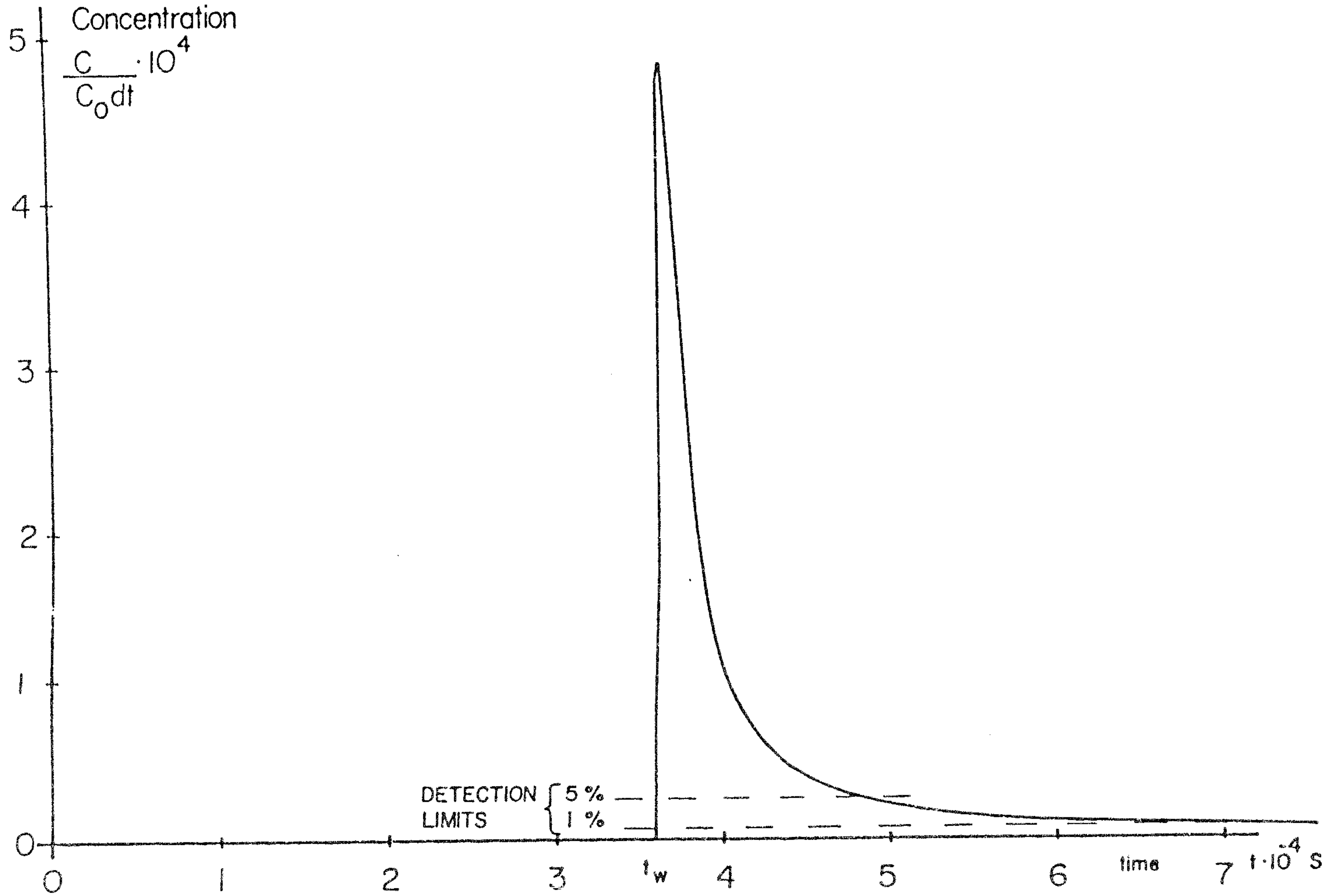

Figure 5 Concentration at the outlet of a single fissure with porous walls. Tracer pulse at the inlet.

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