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Applications of stochastic models to solute transport in fractured rocks

Lynn W Gelhar
Massachusetts Institute of Technology

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SVENSK KÄRNBRÄNSLEHANTERING AB
SWEDISH NUCLEAR FUEL AND WASTE MANAGEMENT CO

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

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ABSTRACT

A stochastic theory for flow and solute transport in a single variable aperture fracture, bounded by a sorbing porous matrix into which solutes may diffuse, is developed using a perturbation approximation and spectral solution techniques which assume local statistical homogeneity. The theory predicts that the effective aperture of the fracture for mean solute displacement will be larger than the aperture required to calculate the large−scale flow resistance of the fracture. This ratio of apertures is a function of the variance of the logarithm of the apertures. The theory also predicts the macrodispersion coefficient for large−scale transport in the fracture. The resulting macrodispersivity is proportional to the variance of the logaperture and to its correlation scale. When variable surface sorption is included, it is found that the macrodispersivity is increased significantly, in some cases more than an order of magnitude. It is also shown that the effective retardation coefficient for the sorptively heterogeneous fracture is found by simply taking the arithmetic mean of the local surface sorption coefficient. Matrix diffusion is also shown to increase the fracture macrodispesivity at very large times. A reexamination of the results of four different field tracer tests in crystalline rock in Sweden and Canada shows aperture ratios and dispersivities that are consistent with the stochastic theory. The variance of the natural logarithm of the aperture is found to be in the range of 3 to 6 and the correlation scales for logaperture ranges from .2 to 1.2 meters. Detailed recommendations for additional field investigations at scales ranging from a few meters up to a kilometer are presented.

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1. INTRODUCTION

The movement of solutes through fractured rocks of relatively low permeability has been the focus of much recent research, largely because of the need to quantify the transport mechanisms in these rocks in terms of their radioactive waste isolation capabilities. Much of the theoretical modeling of fractured rocks has emphasized the flow and transport in networks of individual fractures which are planar and of constant aperture (*Long et al* (1982), *Schwartz et al* (1983), *Robinson* (1984)). Another modeling approach which has been extensively explored since the initial work by *Neretnieks* (1980) is the so-called matrix diffusion model, which considers flow in a single constant aperture fracture with diffusive transport in the surrounding porous but impermeable rock matrix. *Brown and Gelhar* (1986) review the various modeling approaches which have been used for fractured rock transport. Recently *de Marsily* (1985) has suggested a purely geometric network approach based on percolation theory. However, the fact is that there is no established theory which has been shown to be valid for transport in fractured rocks at field scales of tens to thousands of meters.

Recent small-scale field observations by *Abelin et al* (1985) suggest that flow within an individual fracture is limited to a relatively small portion of the fracture plane. This so-called channeling implies that individual fractures cannot be treated as having constant aperture has been done in network models. Recent results from a tracer test which isolated a single fracture (*Lever et al* (1985)) show a large dispersion effect in the single fracture and indicate that the fracture cannot be treated as one of constant aperture. These observations bring into question the basic building block which has been used in all network modeling, i.e. the assumption of a constant aperture planar fracture.

The influence of aperture variation on the flow in the fracture has been explored by *Tsang and Witherspoon* (1981) and *Tsang* (1984). In those studies the aperture is viewed as a random variable and its spatial correlation structure is not considered. *Brown* (1984) developed a stochastic approach which treats flow and solute transport in a planar variable aperture fracture where the aperture variability is characterized by a two-dimensional statistically anisotropic stationary random field.

Stochastic models have been used extensively to treat flow and transport in heterogeneous porous media (*Gelhar and Axness* (1983), *Gelhar* (1984)). These

stochastic theories are now being tested under large-scale field conditions, and initial results (*Sudicky* (1985)) indicate that the stochastic theory can predict field scale dispersivities.

The purposes of this report are to develop a similar stochastic theory for transport in fractured rocks, and to review field observations from tracer tests in fractured rock, particularly those in Sweden, in relation to possible applications of such stochastic theories. First the stochastic theory for transport in a variable aperture fracture is developed. This analysis is an extension of the work of *Brown* (1984) and includes the important influence of the unsteadiness of the solute transport, as well as the effects of spatially variable surface adsorption and diffusion into the porous matrix. The results of several recent tracer tests in fractured rock are analyzed in relation to the predictions of the stochastic theory. These comparisons focus on the dispersion effect of the variable aperture as well as the difference between the effective apertures that must be used for hydraulic and solute transport calculations. The possible application of three-dimensional stochastic theories to large-scale transport in fractured rocks is also discussed briefly. Included are recommendations for additional theoretical developments and field investigations which could be used to evaluate the stochastic approach.

2. STOCHASTIC THEORY OF TRANSPORT IN A SINGLE VARIABLE APERTURE FRACTURE

2.1 General formulation

Consider laminar flow in a single variable aperture fracture which is surrounded by a porous but impermeable rock matrix. The flow configuration is depicted in Figure 1. If the slope of the fracture walls is not large, the local flow through the fracture can be represented by the classical cubic law,

$$Q_i = - \frac{b^2 g}{12 \nu} \frac{\partial \varphi}{\partial x_i}, \quad i = 1,2 \qquad (2.1)$$

where φ = piezometric head [L]

$b(x_1,x_2)$ = fracture aperture [L]

g = gravitational constant [L/T^2]

ν = kinematic viscosity [L^2/T]

x_i = space coordinates in the fracture plane [L]

Q_i = flow per unit width [L^2/T]

As discussed by *Brown* (1984) and *Langlois* (1964), the correction to (2.1) due to the variation in the aperture will be of order the cube of the slope of the aperture, so that it is entirely consistent to neglect this effect in view of later approximations that are introduced in this analysis.

Assuming a rigid fracture and an incompressible fluid (water), conservation of mass of water flowing in a fracture requires that

$$\frac{\partial Q_i}{\partial x_i} = 0 \qquad i = 1,2 \qquad [2.2]$$

The mass balance equation for a solute of a concentration c which is transported by the fluid flowing in the fracture can be written

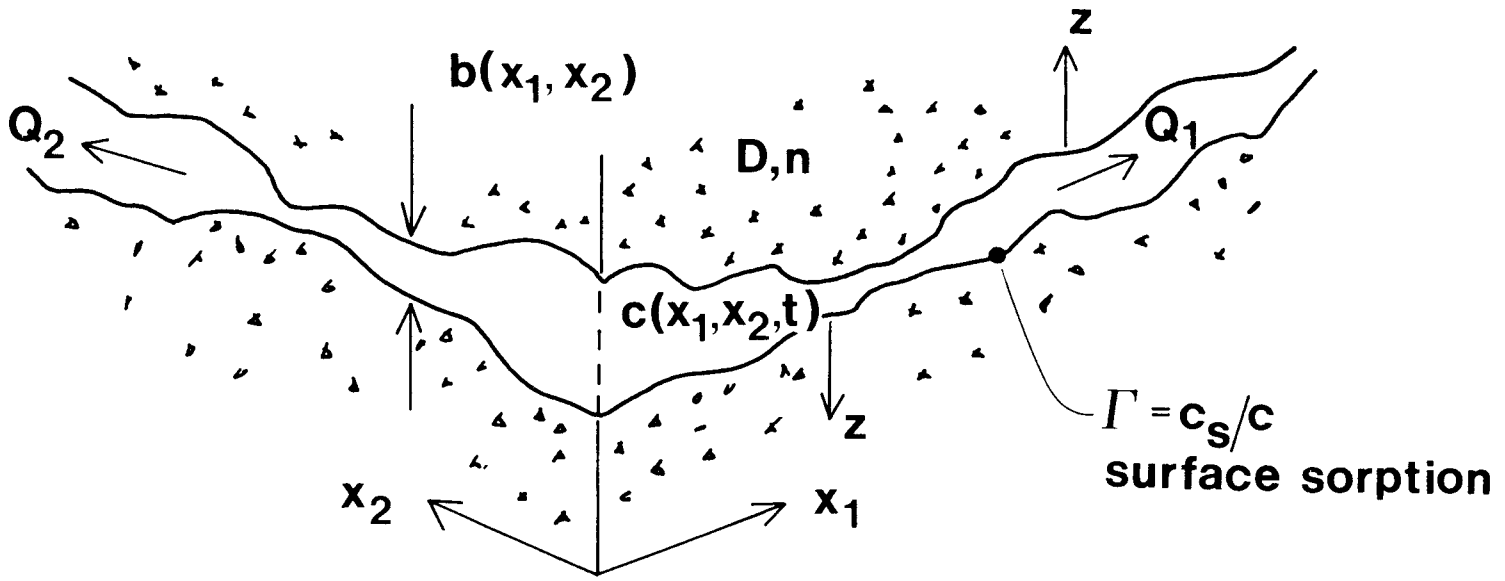

Figure 1 Single variable aperture fracture bounded by a porous matrix with surface sorption.

$$\frac{\partial}{\partial t}(cb) + \frac{\partial}{\partial x_i}(Q_i c) - \frac{\partial}{\partial x_i}\left[E_{ij}\frac{\partial c}{\partial x_j}\right] = -2\Gamma\frac{\partial c}{\partial t} + 2D\left.\frac{\partial m}{\partial z}\right|_{z=0} - r(b + 2\Gamma)c \qquad (2.3)$$

where
- c = concentration in the fracture, $[M/L^3]$
- t = time $[T]$
- E_{ij} = local fracture dispersion coefficient $[L^3/T]$
- Γ = surface sorption coefficient (the ratio of the concentration on the fracture surface to the concentration in the solution in the fracture) $[L]$
- m = concentration in the solution in the porous matrix $[M/L^3]$
- D = effective molecular diffusion coefficient of the porous matrix $[L^2/T]$
- z = distance into porous matrix from the fracture wall $[L]$
- r = first order decay rate constant $[T^{-1}]$

Assuming that the diffusive transport in the static water within the porous matrix is predominantly in the z−direction, the concentration in the porous matrix is described by

$$\frac{\partial m}{\partial t} = D\frac{\partial^2 m}{\partial z^2} - rm \qquad (2.4)$$

where
- D = $D/(n+\rho K_d)$, the effective diffusivity of the porous matrix $[L^2/T]$
- n = porosity of the porous matrix
- ρ = bulk density of the porous matrix $[M/L^3]$
- K_d = distribution coefficient of the porous matrix $[L^3/M]$

In addition, (2.3) and (2.4) are coupled by the following condition

$$c(x_1, x_2, t) = m(z, t; x_1, x_2)\big|_{z=0} \qquad (2.5)$$

Note that x_1 and x_2, the coordinates in the plane of the fracture, appear only parametrically in the balance equation for the porous matrix, (2.4).

Models equivalent to (2.3) through (2.5) have been used by *Neretnieks* (1980) and *Moreno et al* (1983) among others to treat transport in fractures with spatially constant aperture. It is becoming evident from observations and seems obvious based on common sense that the aperture in real fractures is not going to be spatially constant. The focus of the following stochastic analysis is a quantitative evaluation of the effect of variable aperture on the transport process in a fracture. The influence of variable surface sorption and of matrix diffusion will also be analyzed.

To describe the aperture variability, the aperture is treated as a two-dimensional spatial random field. In order to focus on the key elements of the problem a simple statistically isotropic and homogeneous (i.e. stationary) random field is used. The more complicated statistically anisotropic case has been considered by *Brown* (1984) for steady-state solute transport. Here the influence of a time-dependent concentration field is explored, along with the effects of variable surface sorption and matrix diffusion. The overall goal in these analyses is to find effective large-scale transport properties for the heterogeneous fracture system. Before proceeding with the solute transport analysis, it is necessary to develop a description of the spatially-variable flow field that is caused by the aperture variation.

2.2 Flow analysis

This analysis is very similar to that for two-dimensional flow in porous media (*Mizell et al* (1982)) and was developed in detail by *Brown* (1984). Here only the highlights are summarized. First the variables in (2.1) and (2.2) are represented by means and perturbations as follows

$$
\begin{aligned}
Q_i &= \bar{Q}_i + Q_i' \;;\; E(Q_i') = 0 \\
\ln b &\equiv \ln b_g + \beta;\quad E(\beta) = 0 \\
\varphi &= H + h,\; E(h) = 0
\end{aligned}
\qquad (2.6)
$$

By using the logarithm of b, negative values of b are avoided. Using (2.6) in (2.2) it follows that

$$\frac{\partial \bar{Q}_i}{\partial x_i} = 0 \qquad (2.7)$$

which when subtracted from (2.2) leads to

$$\frac{\partial Q'_i}{\partial x_i} = 0 \qquad (2.8)$$

Similarly, the flow equation (2.1) can be written

$$\begin{aligned} Q_i = \bar{Q}_i + Q'_i &= \frac{b_\ell^3 g}{12\nu} e^{3\beta} \left[J_i - \frac{\partial h}{\partial x_i} \right] \\ &= T_\ell \left(1+3\beta + \frac{9}{2}\beta^2 + \ldots\right)\left(J_i - \frac{\partial h}{\partial x_i}\right) \end{aligned} \qquad (2.9)$$

where $T_\ell = b_\ell^3 g/12\nu$, the fracture transmissivity based on the geometric mean aperture, and $J_i = -\partial H/\partial x_i$, the mean hydraulic gradient.

Retaining terms to second order in the perturbations, the mean flow becomes

$$\bar{Q}_i = T_\ell \left[J_i \left(1 + \frac{9}{2}\sigma_\beta^2\right) - 3E\left(\beta \frac{\partial h}{\partial x_i}\right) \right] \qquad (2.10)$$

The last term in (2.10) reflects the correlation between the aperture perturbation and the resulting head perturbation. This term is evaluated by solving for the head perturbation in terms of the aperture perturbation as follows. From (2.9) the flow perturbation can be written, to first order, as

$$Q'_i = T_\ell \left(3J_i \beta - \frac{\partial h}{\partial x_i}\right) \qquad (2.11)$$

and using (2.11) in (2.8), the equation relating the head and aperture perturbation becomes

$$\frac{\partial^2 h}{\partial x_i^2} = 3J_i \frac{\partial \beta}{\partial x_i} \qquad (2.12)$$

This equation can be solved for a stationary head field by using the spectral representation theorem,

$$h = \int_{-\infty}^{\infty} e^{i k_i x_i} \, dZ_h(k_i) \qquad (2.13)$$

where $E[\, dZ_h \, dZ_h^* \,] = S_{hh}(k_i) \, dk_1 \, dk_2$, k_i is the wave number vector, and S_{hh} is the spectral density function for head (the asterisk denotes the complex conjugate).

The corresponding representation for the logaperture perturbation is

$$\beta = \int_{-\infty}^{\infty} e^{i k_i x_i} \, dZ_\beta(k_i) \qquad (2.14)$$

and using (2.13) and (2.14) in (2.12), along with the uniqueness of these representations, it follows that

$$- k^2 \, dZ_h = 3 i \, J_j \, k_j \, dZ_\beta \qquad (2.15)$$

The cross-correlation term in (2.10) is then evaluated as follows

$$\begin{aligned} E\left[\beta \frac{\partial h}{\partial x_i}\right] &= \int_{-\infty}^{\infty} E[\, dZ_\beta(- i k_i) \, dZ_h^* \,] \\ &= \int_{-\infty}^{\infty} 3 J_j \frac{k_i k_j}{k^2} S_{\beta\beta}(k) \, dk_1 \, dk_2 \\ &= 3 J_j \delta_{ij} \sigma_\beta^2 / 2 \end{aligned} \qquad (2.16)$$

where $\delta_{ij} = 1$ if $i = j$ and 0 if $i \neq j$, and $\sigma_\beta^2 = E(\beta^2)$, the variance of ln b.

This result makes use of the assumption that the logaperture field is isotropic, and therefore that its spectral density function is dependent on only the magnitude of the wave number k. Note that this result does not depend on the

specific form of the spectral density function of ln b, or equivalently, on the covariance function or its correlation scale.

Using (2.16) in (2.10), the mean flow becomes

$$Q_i = T_\ell \, J_i ; \quad T_\ell = b_\ell^3 \, g/12\nu \tag{2.17}$$

That is, the effective transmissivity of the fracture is determined simply by using the geometric mean aperture in the cubic law. This result is equivalent to those of *Gutjahr et al* (1978) and *Dagan* (1979) for two-dimensional flow and statistically isotropic porous media. *Brown* (1984) has developed more general results for the statistically anisotropic case. These give relationships for the degree of anisotropy of the fracture transmissivity in terms of the ratio of the two correlation scales.

The flow perturbation, after using the representation theorem, can be expressed in terms of the aperture perturbation by using (2.15) in (2.11)

$$\begin{aligned} dZ_{Q_i} &= T_\ell (3J_i \, dZ_\beta - ik_i dZ_h) \\ &= 3T_\ell \, J_j \left[\delta_{ij} - \frac{k_i \, k_j}{k^2}\right] dZ_\beta \end{aligned} \tag{2.18}$$

This relationship is important in the transport analysis which follows.

2.3 Unsteady transport with no sorption and diffusion

Using $\Gamma = D = 0$ in (2.3) and expressing the concentration in terms of the mean and perturbation,

$$c = \bar{c} + c', \quad E(c) = \bar{c}, \quad E(c') = 0 \tag{2.19}$$

the mean transport equation becomes, after taking the expected value,

$$\bar{b}\,\frac{\partial \bar{c}}{\partial t} + E\left[b'\,\frac{\partial c'}{\partial t}\right] + \bar{Q}_i\,\frac{\partial \bar{c}}{\partial x_i} + E\left[Q_i'\,\frac{\partial c'}{\partial x_i}\right] - E\,\frac{\partial^2 \bar{c}}{\partial x_c^2}$$

$$+ r[\bar{b}\,\bar{c} + E(b'c')] = 0 \qquad (2.20)$$

where $E_{ij} = E\,\delta_{ij}$, E = constant.

Note that the local fracture dispersion term has been treated as a constant, say corresponding to molecular diffusion. The influence of variable local dispersion can also be analyzed, but its effect is easily shown to be secondary. The terms involving products of perturbations in (2.20) must be evaluated in order to determine the mean behavior. To evaluate these terms the solution for the concentration perturbation must be found. By subtracting (2.20) from (2.3) the equation for the concentration perturbation can be written

$$b'\,\frac{\partial \bar{c}}{\partial t} + \bar{b}\,\frac{\partial c'}{\partial t} + Q_i'\,\frac{\partial \bar{c}}{\partial x_i} + \bar{Q}_i\,\frac{\partial c'}{\partial x_i} - E\,\frac{\partial^2 c'}{\partial x_i^2} + r(\bar{b}c' + \bar{c}b')$$

$$= 0 \qquad (2.21)$$

This expression is valid to first order in perturbations. In order to correctly capture the effect of an unsteady mean concentration field it is necessary to express (2.20) and (2.21) in a moving coordinate system which translates with the mean advection velocity, V. For convenience select the coordinate system so that the mean flow is in the x_1 direction, that is,

$$\bar{Q}_1 = Q,\ \bar{Q}_2 = 0$$

The moving coordinate system can then be expressed as

$$\xi_1 = x_1 - Vt;\quad \xi_2 = x_2 \qquad (2.22)$$

The mean advection velocity is not known at this stage but will be determined by evaluating the cross-correlation terms in (2.20). In this moving coordinate system, which corresponds to riding along with a moving front or a pulse of solute, the mean concentration gradient will vary slowly in time. Writing the mean and perturbation equations, (2.20) and (2.21), in moving coordinate system,

$$\bar{b}\left.\frac{\partial \bar{c}}{\partial t}\right|_{\xi_i} + (Q - \bar{b}V)\frac{\partial \bar{c}}{\partial \xi_1} - E\frac{\partial^2 \bar{c}}{\partial \xi_i^2} + \left.\frac{\partial}{\partial t}\overline{b'c'}\right|_{\xi_i} -$$

$$- V\frac{\partial}{\partial \xi_1}\overline{b'c'} + \frac{\partial}{\partial \xi_i}\overline{c'Q_i'} + r(\bar{b}\bar{c} + \overline{b'c'}) = 0 \qquad (2.23)$$

$$\left[\left.\frac{\partial \bar{c}}{\partial t}\right|_{\xi_i} - V\frac{\partial \bar{c}}{\partial \xi_1}\right] b' + \bar{b}\left.\frac{\partial c'}{\partial t}\right|_{\xi_i} + (Q - V\bar{b})\frac{\partial c'}{\partial \xi_i} +$$

$$+ Q_i'\frac{\partial \bar{c}}{\partial \xi_i} - E\frac{\partial^2 c'}{\partial \xi_i^2} + r\bar{b}c' + r\bar{c}b' = 0 \qquad (2.24)$$

where now $\bar{c}_i = \bar{c}_i(\xi_i, t)$ and $c_i' = c_i'(\xi_i, t)$. Also used in (2.23) is the fact that

$$\overline{b'\left.\frac{\partial c'}{\partial t}\right|_{x_i}} = \frac{\partial}{\partial t}\left(\overline{b'c'}\right)\Big|_{x_i}$$

because the aperture is not time dependent.

Note that the overbars denote expected values. The terms $\overline{b'c'}$ and $\overline{Q_i'c'}$ in (2.23) will now be related to the mean concentration field through the solution for the concentration perturbation.

Consider situations in which the mean concentration field is dispersed over an area much larger than the correlation scale of the aperture variation. In this situation the concentration gradient can be viewed as being locally constant, in which case a locally stationary solution for the concentration perturbation is possible according to (2.24). Thus the concentration perturbation is represented by

$$c' = \int_{-\infty}^{\infty} e^{ik_i x_i}\, dZ_c$$

$$= \int_{-\infty}^{\infty} e^{i[k_1(\xi_1 + Vt) + k_2\xi_2]}\, dZ_c(k_i;\ t) \qquad (2.25)$$

where the second line in (2.25) is used when the concentration is described in the moving coordinate system. Using (2.25) and the representation of b'

$$b' = \int_{-\infty}^{\infty} e^{i\, k_i x_i}\, dZ_b(k_i) \qquad (2.26)$$

the equation for the concentration amplitude becomes

$$\bar{b}\, \frac{\partial F}{\partial t}\Big|_{\xi_i} + (ik_1 Q + Ek_i^2 + r\bar{b})F = G_j\, dZ_{Q_j} - (\dot{\bar{c}} + \bar{c}r)\, dZ_b \qquad (2.27)$$

where $F = dZ_c$, $G_j = -\partial\bar{c}/\partial\xi_j$, and

$$\dot{\bar{c}} = \frac{\partial\bar{c}}{\partial t}\Big|_{\xi_i} - V\,\frac{\partial\bar{c}}{\partial\xi_1} = \frac{\partial\bar{c}}{\partial t}\Big|_{\xi_i} + VG_1 \qquad (2.28)$$

which is treated as being locally constant in relation to the perturbation equation.

For large time and large displacement, the time derivative in (2.27) becomes small and

$$dZ_c = [G_j\, dZ_{Q_j} - w\, dZ_b\,]/\Omega \qquad (2.29)$$

$$\Omega = ik_1 Q + Ek_i^2 + r\bar{b}$$

$$w = \dot{\bar{c}} + r\bar{c} = VG_1 + \partial\bar{c}/\partial t\,|_{\xi_i} + r\bar{c}$$

$$\cong VG_1 + r\bar{c}$$

Gelhar (1986) has explicitly analyzed the effect of the transient term for the case of three-dimensional flow in porous media. For this large time asymptotic condition it is also consistent to neglect the time derivative of the mean concentration following the mean advection in w, because this term is easily shown to be much smaller than the term VG_1. The cross-correlation terms in the mean equation (2.23) can now be evaluated. Only longitudinal dispersion will be treated here, so that only the following terms are considered.

$$dZ_c = G_1(dZ_{Q_1} - VdZ_b)/\Omega - r\bar{c}\, dZ_b/\Omega \qquad (2.30)$$

Also in (2.23) the following term

$$\frac{\partial}{\partial t}\overline{b'c'}\Big|_{\xi_i}$$

is also small and introduces only high order derivatives of the mean concentration in the mean equation. Therefore the two terms

$$\frac{\partial}{\partial \xi_1}\overline{c'Q_1'} - V\frac{\partial}{\partial \xi_1}\overline{c'b'} = \frac{\partial}{\partial \xi_1}\overline{c'(Q_1' - Vb')} \qquad (2.31)$$

are the only terms in the mean equation which will produce a second derivative of the mean concentration, that is, a macrodispersion effect. These terms are evaluated as

$$\overline{c'(Q_1' - Vb')} = \int_{-\infty}^{\infty} dZ_c\,(dZ^*_{Q_1} - VdZ^*_b)$$

$$= G_1\int_{-\infty}^{\infty}\overline{(dZ_y\, dZ^*_y/\Omega)} - r\bar{c}\int_{-\infty}^{\infty}\overline{(dZ_y\, dZ^*_b/\Omega)} \qquad (2.32)$$

where $y = Q_1' - Vb'$, $dZ_y = dZ_{Q_i} - VdZ_b$.

Integrals of the type appearing in (2.32) have been evaluated exactly by *Gelhar and Axness* (1983). Here a simple approximate solution which captures the essential behavior of the integral is used. *Gelhar and Axness* (1983) have shown that the local dispersion term has a very small effect on the macrodispersion and may cause a very slight decrease in the overall dispersion effect. Here the local dispersion is simply set equal to zero and the effect of a small radioactive decay term r is considered. Then the first integral on the left hand side of (2.32) can be written

$$\int_{-\infty}^{\infty}\int \frac{S_{yy}(k_1,k_2)\,dk_1dk_2}{(ik_1Q + r\bar{b})} = \int_{-\infty}^{\infty}\int \frac{S_{yy}(r\bar{b} - ik_1Q)}{k_1^2Q^2 + r^2\bar{b}^2}\,dk_1dk_2$$

$$= \int_{-\infty}^{\infty}\int \frac{S_{yy}\left[\frac{r\bar{b}}{Q}v, k_2\right]}{Q(1+v^2)}\,dv\,dk_2 = \frac{\pi}{Q}\int_{-\infty}^{\infty} S_{yy}(0,k_2)\,dk_2 \qquad (2.33)$$

for $r \to 0$ where $v = k_1Q/r\bar{b}$.

The imaginary term in the integral cancels out because the spectrum S_{yy} is even in k_1 and the last expression is obtained in the limit as r becomes very small, that is, when

$$r\bar{b}/Q << \lambda$$

where λ is a correlation scale associated with the spectrum $S_{\beta\beta}$.

Physically this corresponds to a small amount of decay during the period of time that the solute moves one correlation scale. As r goes to zero, the second term on the right hand side of (2.32) disappears, as does the last term in the mean equation (2.23). That is, the mean equation reduces to the form

$$\bar{b}\frac{\partial\bar{c}}{\partial t} + (Q - V\bar{b})\frac{\partial\bar{c}}{\partial\xi_1} - B\frac{\partial^2\bar{c}}{\partial\xi_1^2} = 0 \qquad (2.34)$$

in which only longitudinal mean concentration gradients are included. The term B is the fracture macrodispersion coefficient which is given by the integral in (2.33):

$$B = \frac{\pi}{Q} \int_{-\infty}^{\infty} S_{yy}(0,k_2)\, dk_2 \qquad (2.35)$$

The coefficient of the advection term in (2.34) must, by definition, be zero because V was defined to be the mean advection velocity. Therefore we have the simple common sense result that

$$V = Q/\bar{b} \qquad (2.36)$$

Thus the average advection velocity of a nonreactive solute is simply the flux through the fracture divided by the average fracture aperture. Note that if the radioactive decay terms had been retained in (2.32) and (2.23) there would be an additional first derivative term in the mean transport equation and, as a result, a correction to the mean advection velocity.

To evaluate the fracture macrodispersivity, y is represented by

$$dZ_y = dZ_{Q_1} - V dZ_b$$

$$= 3T_\ell J_1 \left(1 - \frac{k_1^2}{k^2}\right) dZ_\beta - V dZ_b \qquad (2.37)$$

where (2.18) has been used for dZ_{Q_1} with the mean hydraulic gradient in the x_1-direction. Using the relationship for Q in (2.17) and evaluating (2.37) for $k_1 = 0$,

$$dZ_y(0,k_2) = Q(3dZ_\beta(0,k_2) - dZ_b(0,k_2)/\bar{b}) \qquad (2.38)$$

The spectrum required in (2.35) is then found by taking the expected value of (2.38) multiplied by its complex conjugate. Note that the resulting spectrum will depend on the spectrum of the logaperture process and the spectrum of the aperture process. These two spectra are not the same in general. However, if b is lognormal it is possible to relate the covariance function of the aperture to the covariance function of the logaperture as discussed by *Gutjahr et al* (1978). They show that the covariance function of b can be related to the covariance function of β by the following

$$R_{bb} = \sigma_b^2 \frac{[\exp(R_{\beta\beta}) - 1]}{\exp(\sigma_\beta^2) - 1} \qquad (2.39)$$

The existence of this relationship then implies that the spectra are related to a transfer function relationship of the form

$$dZ_b = H(k_1, k_2)\, dZ_\beta \qquad (2.40)$$

where H is the transfer function. Equation (2.38) leads to the spectral relationship

$$\begin{aligned} S_{yy} &= Q^2(9\, S_{\beta\beta} - 6\, S_{\beta b}/\bar{b} + S_{bb}/\bar{b}^2) \qquad (2.41) \\ &= Q^2(3 - H/\bar{b})^2\, S_{\beta\beta} \end{aligned}$$

where $S_{\beta b}$ is the crosspectrum between β and b, and (2.40) has been used. An approximate relationship will be developed to account for the influence of nonlinear relationship between logaperture and aperture as follows. First the spectrum of logaperture is assumed to be that corresponding to an exponential covariance

$$S_{\beta\beta} = \frac{Q_\beta^2\, \lambda^2}{2\pi\, [1 + \lambda^2(k_1^2 + k_2^2)]^{3/2}} \qquad (2.42)$$

and

$$\int_{-\infty}^{\infty} S_{\beta\beta}(0, k_2)\, dk_2 = \sigma_\beta^2\, \lambda/\pi \qquad (2.43)$$

where λ is the correlation scale. This gives the contribution of the first term in (2.41) to the macrodispersion coefficient in (2.35). For the last term in (2.41) it would be assumed that a similar relationship applies but that the variance and the correlation scale of b appear in the expression, and the middle term involving the crosspectum in (2.41) will be assumed to be the result of forming the square of the difference. Then the integral from (2.35) can be approximated as

$$B = Q(3\sigma_\beta\sqrt{\lambda} - \sigma_b\sqrt{\lambda_b}/\bar{b})^2 \qquad (2.44)$$

$$= Q\,\sigma_\beta^2\,\lambda\,(3-f)^2$$

where $f = (\sigma_b/\bar{b}\;\sigma_\beta)\sqrt{\lambda_b/\lambda}$.

For a lognormal distribution

$$\sigma_b/\bar{b} = (e^{\sigma_\beta^2} - 1)^{1/2} \qquad (2.45)$$

and by assuming that $R_{bb}(\lambda_b)/\sigma_b^2 = e^{-1}$ in (2.39),

$$\frac{\lambda_b}{\lambda} = -\ell n\left[\frac{1}{\sigma_\beta^2}\,\ell n\left[\frac{e^{\sigma_\beta^2}-1}{e} + 1\right]\right] \qquad (2.46)$$

From (2.46) it can be seen that the correlation scale for the aperture will be less than that for the logaperture, and that this difference increases as σ_β increases. From (2.45) and (2.46) it is seen that f in (2.44) will be a function of $\sigma_\beta{}^2$; when the logaperture variance $\sigma_\beta{}^2$ is small f approaches 1 and as $\sigma_\beta{}^2$ increases f increases, for example, to 3 at $\sigma_\beta{}^2 = 5.5$. Therefore this term will have a numerically significant effect on the predicted macrodispersion coefficient in the likely range of $\sigma_\beta{}^2$.

If the mean equation (2.34) is then divided by $\bar{b}$, the dispersion coefficient term has the form

$$B/\bar{b} = (Q/\bar{b})\;\sigma_\beta^2\;\lambda(3-f)^2 = VA \qquad (2.47)$$

using the advection velocity from (2.36). Here A is the fracture dispersivity

$$A = \sigma_\beta^2\;\lambda(3-f)^2 \qquad (2.48)$$

This form is similar to the macrodispersivity for a two-dimensional porous medium flow (*Gelhar and Axness* (1983), equation 71 with $\lambda_1 = \lambda_2$). However, here there is an important difference in that the influence of the variation of

fracture aperture produces the term f in (2.48) and significantly modifies the magnitude of the dispersivity. Note that this result indicates that the dispersivity is a fracture property, i.e., it is not velocity dependent as would be the case if a Taylor−type dispersion model were used. In that case the dispersion coefficient depends on the square of the velocity, so that the dispersivity increases as the first power of velocity.

The two key results of this development are (2.36), the expression for the mean advection velocity, and (2.48), the macrodispersivity of the fracture. These relationships will be used later in interpretation of some of the tracer tests.

The flow analysis showed that the effective hydraulic aperture of the fracture is the geometric mean (see (2.17)), whereas for the transport analysis the aperture which produces the mean advection velocity is the arithmetic mean. For a lognormal distribution, the ratio of geometric and arithmetic means is

$$b_g/\bar{b} = e^{\sigma_\beta^2/2} \qquad (2.49)$$

$$= b_h/b_c$$

where b_h designates the hydraulic aperture which would be calculated from the classical cubic law in a hydraulic experiment where the flow rate and the pressure gradient are measured, and the b_c designates the aperture that would be determined from a tracer test in which the volumetric flow rate and the mean residence time are observed.

2.4 Variable surface sorption

The case of variable surface sorption can be treated as a relatively simple extension of the analyses in Section 2.3 if it is noted that the transport equation (2.3) can be written for the nondiffusive case as

$$(b+2\Gamma)\frac{\partial c}{\partial t} + Q_i\frac{\partial c}{\partial x_i} - \frac{\partial}{\partial x_i}\left(E_{ij}\frac{\partial c}{\partial x_j}\right) + r(b+2\Gamma)c = 0 \qquad (2.50)$$

The sorption term always appears as a term added to b. This combination can then be used as a modified aperture,

$$\theta = b + 2\Gamma \tag{2.51}$$

and the previous analysis is revised as follows. As illustrated in Figure 2, the variation in Γ will not in general be perfectly correlated with that of b; one may expect the relationship of the form

$$\Gamma = \Gamma_o + \zeta b + \eta \tag{2.52}$$

Here Γ_0 and ζ are constants and η is a zero mean residual noise term which is not correlated with b, i.e.,

$$E(\eta) = 0, \quad E(b\eta) = 0 \tag{2.53}$$

Equation (2.52) can be viewed as a linear regression between Γ and b where η is the residual. With this relationship the perturbation in θ can be written as

$$\theta' = (1+2\zeta)b' + 2\eta \tag{2.54}$$

The analysis then proceeds exactly as in Section 2.3 with b' replaced by θ'. Essentially all the terms involving b' are multiplied by $1+2\zeta$. The noise term simply adds an additional independent contribution to the dispersivity. The result for the mean transport equation analogous to (2.34) is

$$\bar{\theta} \frac{\partial \bar{c}}{\partial t} + (Q - V\bar{\theta}) \frac{\partial \bar{c}}{\partial \xi_1} - B \frac{\partial^2 \bar{c}}{\partial \xi_1^2} = 0 \tag{2.55}$$

where V is the mean advection velocity of the solute and

$$B = Q \sigma_\beta^2 \lambda \left[3 - (1+2\zeta) f\bar{b}/\bar{\theta} \right]^2 + 4V^2 \sigma_\eta^2 \lambda_\eta / Q \tag{2.56}$$

where σ_η^2 and λ_η are the variance and correlation scale of the η process, which is assumed to have an exponential covariance with a spectra of the form

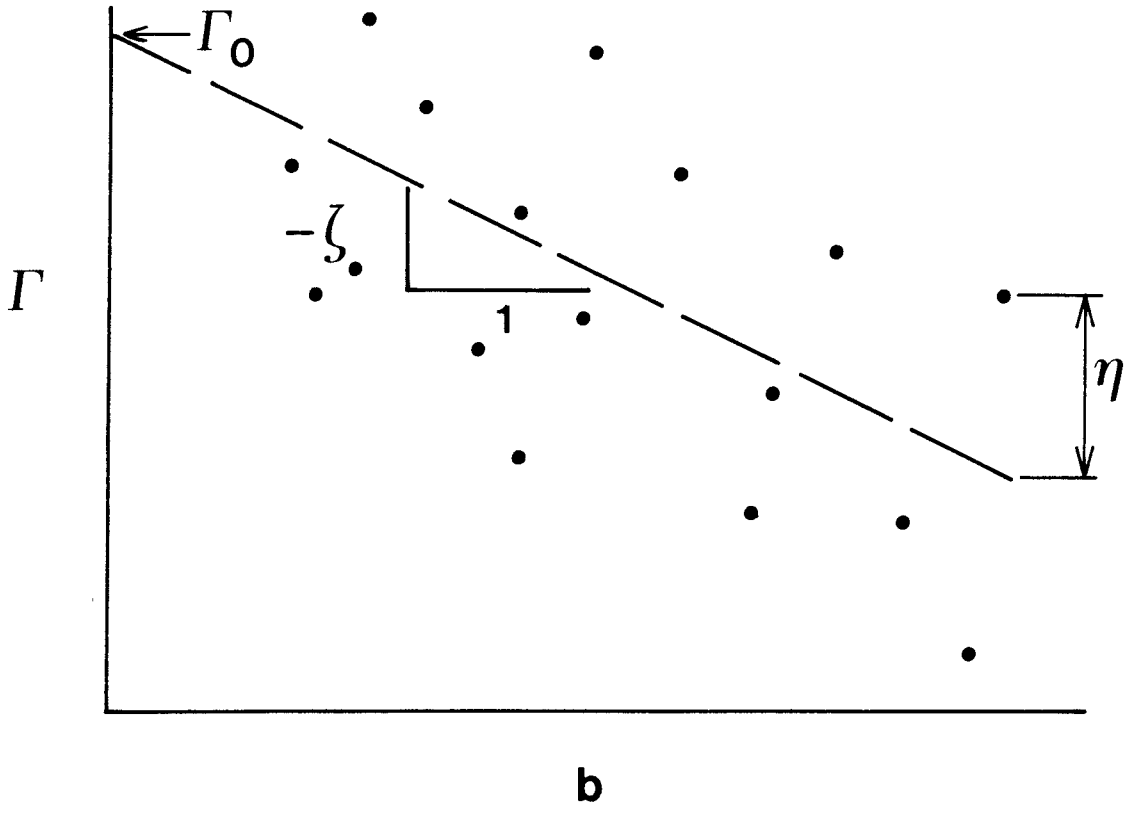

Figure 2 Relationship between surface sorption coefficient Γ and aperture b; Γ_o and ζ are constants.

of (2.42). Again the advection term in the moving coordinate system must disappear so that

$$V = \frac{Q}{\bar{\theta}} = \frac{Q}{\bar{b} + 2\bar{\Gamma}} = \frac{Q}{\bar{b}\ R} \qquad (2.57)$$

where $R = 1 + 2\bar{\Gamma}/\bar{b}$ is the retardation factor.

This is an important result in that it demonstrates that the effective surface sorption coefficient is just the arithmetic mean.

The fracture macrodispersivity is found from (2.56) in the form

$$A = B/\bar{\theta}\ V = \sigma_\beta^2\ \lambda\left[3-(1+2\zeta)f/R\right]^2 + 4\sigma_\eta^2\ \lambda_\eta/\bar{\theta}^2 \qquad (2.58)$$

Note that the resulting macrodispersivity with a variable surface sorption is not the same as that for the nonreactive case. The uncorrelated noise term will always increase the dispersivity whereas the correlated effect may increase or decrease the dispersivity depending on the sign of ζ, and the magnitude of f and the retardation factor.

2.5 Matrix diffusion effects

Here a simplified analysis is developed to demonstrate the influence that matrix diffusion will have on the macrodispersion process in a variable-aperture fracture. Before proceeding with the stochastic analysis some elementary, but apparently not well known, features of the classical deterministic matrix diffusion model will be explored because these features are used to develop the stochastic approach.

The classical matrix diffusion model for a constant aperture fracture is obtained from (2.3) by taking the parameters to be constants. Here the case with no surface sorption ($\Gamma = 0$) or radioactive decay ($r = 0$) will be considered, and the model takes the form

$$\frac{\partial c}{\partial t} + U \frac{\partial c}{\partial x} - D_f \frac{\partial^2 c}{\partial x^2} = \frac{2D}{b} \frac{\partial m}{\partial z}\Big|_{z=0} \qquad (2.59)$$

where $U = Q/b$, and $D_f = E/b$ is the dispersion coefficient of the fracture (a constant).

Only one-dimensional transport is considered. Diffusive transport in the porous matrix is described by (2.4) with $r = 0$, i.e.,

$$\frac{\partial m}{\partial t} = D \frac{\partial^2 m}{\partial z^2} \qquad (2.60)$$

which must satisfy the condition that

$$m(0,t) = c(x,t) \qquad (2.61)$$

In order to visualize the influence of matrix diffusion, it is convenient to express the term involving m in (2.59) in terms of the concentration c in the fracture. That can be done by noting that a general solution to (2.60) which satisfies (2.61) is

$$m(z,t) = \int_{\tau=0}^{t} \frac{\partial c}{\partial t}\Big|_{t=\tau} \operatorname{erfc}\left[\frac{z}{\sqrt{4D(t-\tau)}}\right] d\tau \qquad (2.62)$$

and evaluating the derivative at $c = 0$,

$$\frac{\partial m}{\partial z}\Big|_{z=0} = -\int_{\tau=0}^{t} \frac{\partial c}{\partial t}\Big|_{t=\tau} \frac{d\tau}{\sqrt{\pi D(t-\tau)}} \qquad (2.63)$$

$$\cong -\left[\frac{\partial c}{\partial t}\int_{\tau=0}^{t} \frac{dt}{\sqrt{\pi D(t-\tau)}} - \frac{\partial^2 c}{\partial t^2}\int_{\tau=0}^{t} \frac{(t-\tau)\,d\tau}{\sqrt{\pi D(t-\tau)}} + \ldots\right]$$

$$= -\frac{2}{\sqrt{\pi D}}\left[\sqrt{t}\,\frac{\partial c}{\partial t} - t^{3/2}\frac{\partial^2 c}{\partial t^2} + \ldots\right]$$

where the approximate expressions on the last two lines have been obtained by expanding $\partial c/\partial t$ around the point $t = \tau$, that being the area of dominant contribution to the integral. Using the last line of (2.63) in (2.59),

$$\frac{\partial c}{\partial t} + U \frac{\partial c}{\partial x} - D_f \frac{\partial^2 c}{\partial x^2} \cong \frac{4}{b} \sqrt{\frac{Dnt}{\pi}} \left[- \frac{\partial c}{\partial t} + t \frac{\partial^2 c}{\partial t^2} \right] \qquad (2.64)$$

where it has been assumed that there is no sorption in the matrix. Equation (2.64) demonstrates, in a simple approximate form, the influence of matrix diffusion. The term involving the first derivative in time on the right hand side of (2.64) can be seen as a time-varying retardation effect due to matrix diffusion, whereas the second derivative in time can be shown, by substituting $\partial c/\partial t$ from the left side of the equation, to produce a term involving a second derivative in the space coordinate, i.e., an additional dispersion effect due to matrix diffusion.

The relative importance of matrix diffusion is reflected by the time dependent coefficient multiplying the right hand side of (2.64). Physically this can be recognized as the ratio of a diffusion thickness

$$\delta = 4\sqrt{Dnt/\pi} \qquad (2.65)$$

to the fracture aperture. When the δ/b is large, the matrix diffusion effect is dominant. In that case it is easily shown that the second derivative term leads to an additional dispersion effect which is proportional to

$$\frac{V^2 b^2}{Dn} \cdot \frac{\delta}{b}$$

which is in the form of a Taylor dispersion coefficient but, in this case, increases as the square root of time because of the factor δ/b. The above features of retardation and additional dispersion due to matrix diffusion can also be verified by taking the first and second spatial moments of the concentration from the exact solution for a pulse input with no fracture dispersion as given by *Neretnieks* (1980).

The primary influence of matrix diffusion in terms of the stochastic analyses of a variable aperture fracture will be through the retardation term associated with

the first derivative on the right hand side of (2.64). The resulting mean advection velocity of a solute is

$$V = U/(1+\delta/b) = Q/(b+\delta)$$

This feature will be incorporated in the stochastic analysis which follows.

The stochastic analysis of the variable aperture situation is again very similar to the development in Section 2.3. The model equation to be used in this analysis is based on (2.3) with the matrix diffusion term approximated as discussed above.

$$b\,\frac{\partial c}{\partial t} + Q_i\,\frac{\partial c}{\partial x_i} - E\,\frac{\partial^2 c}{\partial x_i^2} \cong -\,\delta\,\frac{\partial c}{\partial t} \qquad (2.66)$$

Here only the first derivative in time from (2.64) has been included because it is easily shown that the second derivative does not affect the evaluation of the storage or dispersion terms in the mean equation. Under this condition the influence of matrix diffusion on the mixing process in the variable aperture fracture is a very simple one which is represented by an additional time dependent storage term, that is, the term δ in (2.65). The method of analysis and results from Section 2.3 can then be applied directly by replacing b by $b+\delta$. Note here that the local dispersion term in a fracture has been retained but that the radioactive decay term is omitted. The analysis proceeds with exactly the same steps as in Section 2.3 except for the evaluation of the integral in (2.33), which differs because now the fracture dispersion term has been retained. That integral is evaluated as follows

$$\int_{-\infty}^{\infty}\int \frac{S_{yy}(k_1,k_2)\,dk_1\,dk_2}{i\,k_1 Q + E\,k_i^2} = \int_{-\infty}^{\infty}\int \frac{S_{yy}\,k_i^2\,E}{k_1^2 Q_1^2 + E^2(k_i^2)^2}\,dk_1 dk_2$$

$$= \frac{1}{Q}\int_{-\infty}^{\infty}\int \frac{S_{yy}(Ev/Q,k_2)\;(E^2v^2/Q^2 + k_2^2)}{v^2 + (E^2v^2/Q^2 + k_2^2)}\,dvdk_2$$

$$= \frac{1}{Q}\int_{-\infty}^{\infty}\int \frac{S_{yy}(0,k_2)\,k_2^2}{v^2 + k_2^2}\,dvdk_2 = \frac{\pi}{Q}\int_{-\infty}^{\infty} S_{yy}\,(0,k_2)dk_2 \qquad (2.67)$$

for $E \to 0$, i.e., $E/Q\lambda << 1$. If $E = D\bar{b}$, $E/Q\lambda$ is on the order of 10^{-4} so that molecular diffusion has no effect on the macrodispersion.

If Taylor dispersion is considered in the fracture, that ratio will still be small for apertures as large as a millimeter.

The results for the case with matrix diffusion are found simply by replacing b by $b+\delta$ in the results in Section 2.3. Then the average advection velocity of a solute becomes, from (2.36),

$$V = Q/(\bar{b}+\delta) \tag{2.68}$$

and when this velocity is used in the development for the macrodispersion coefficient, (2.44) is replaced by

$$B = Q\,\sigma_\beta^2\,\lambda(3-\hat{f})^2 \tag{2.69}$$

$$\text{where } \hat{f} = [\sigma_b/(\bar{b}+\delta)\sigma_\beta]\sqrt{\lambda_b/\lambda} = f \cdot \frac{\bar{b}}{\bar{b}+\delta}$$

Therefore the effect of matrix diffusion on the macrodispersion coefficient is to produce a coefficient which will increase slowly with time because of the added δ term in f.

The above macrodispersion term is then incorporated in the mean transport equation with matrix diffusion as follows

$$\bar{b}\,\frac{\partial \bar{c}}{\partial t} + Q\,\frac{\partial \bar{c}}{\partial x_i} - (E + B)\,\frac{\partial^2 \bar{c}}{\partial x_i^2} = 2D\,\frac{\partial \bar{m}}{\partial z}\bigg|_{z=0} \tag{2.70}$$

with $\bar{m} = \bar{c}$ at $z = 0$ and

$$\frac{\partial \bar{m}}{\partial t} = D\,\frac{\partial^2 \bar{m}}{\partial z^2}, \quad D = D/n \tag{2.71}$$

This of course is the classical matrix diffusion model except that the macrodispersion coefficient is a function of time according to (2.69). Existing analytical and numerical solutions of this system can be used in applications.

2.6 Discussion and results

Several important new results have been developed in the previous sections. First of all, it has been shown that the stochastic theory provides a unified quantitative explanation of both the channeling effect that has been observed in natural fractures and the macrodispersion effect of the aperture variability. The channeling effect is reflected in the ratio of the hydraulic aperture to the solute aperture (see (2.49)) and the dispersion effect is predicted by (2.48), which shows the dependence of the fracture macrodispersivity on the variance and correlation scale of the logaperture process. The factor f in (2.48) reflects the effect of the aperture variation through the storage term in the unsteady transport equation. This effect is quantitatively very important and reduces the dispersivity. This behavior differs significantly from the porous medium case where the analogous variation in porosity produces only a minor effect.

When surface sorption is included in the analysis (Section 2.4), it is found that there are significant changes in the nature of the result. First of all, it is shown that the effective retardation coefficient for a spatially variable surface sorption coefficient can be found simply by taking the arithmetic mean of the variable surface sorption coefficient (see (2.57)). This is a simple but very important observation because it provides a sound basis for estimating large scale retardation coefficients from a number of small scale measurements. It is also found that the sorption process has a very significant effect on the macrodispersivity of the fracture. This is reflected in (2.58) which shows that the dispersivity can increase significantly with increasing retardation coefficient. This effect is illustrated in Figure 3 which shows macrodispersivities calculated for sorbing and nonsorbing solutes.

When the effect of matrix diffusion was included (Section 2.5), it was found, using an approximate analysis which incorporates the effect of matrix diffusion in the concentration perturbation equation through a time−varying retardation effect, that the fracture macrodispersivity is significantly affected by matrix diffusion. In this case the result is a time varying macrodispersion coefficient which increases with time (see (2.69)). This effect is illustrated graphically in Figure 4. Note

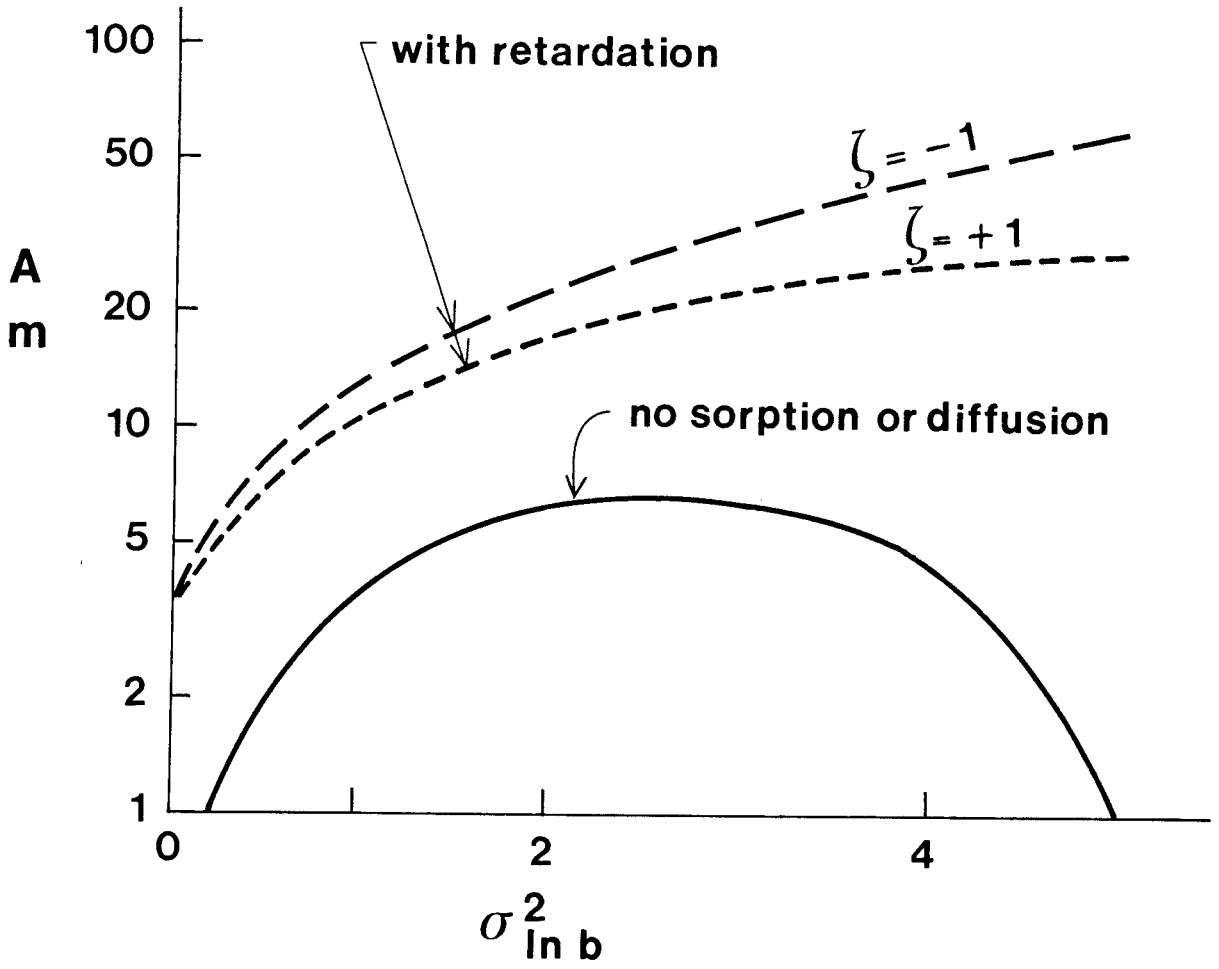

Figure 3 Fracture macrodispersivity for sorbing and nonsorbing solutes; for $\lambda = \lambda_\eta = 1$ m, $\sigma_\eta/\bar{\Gamma} = 1$, R = 10.

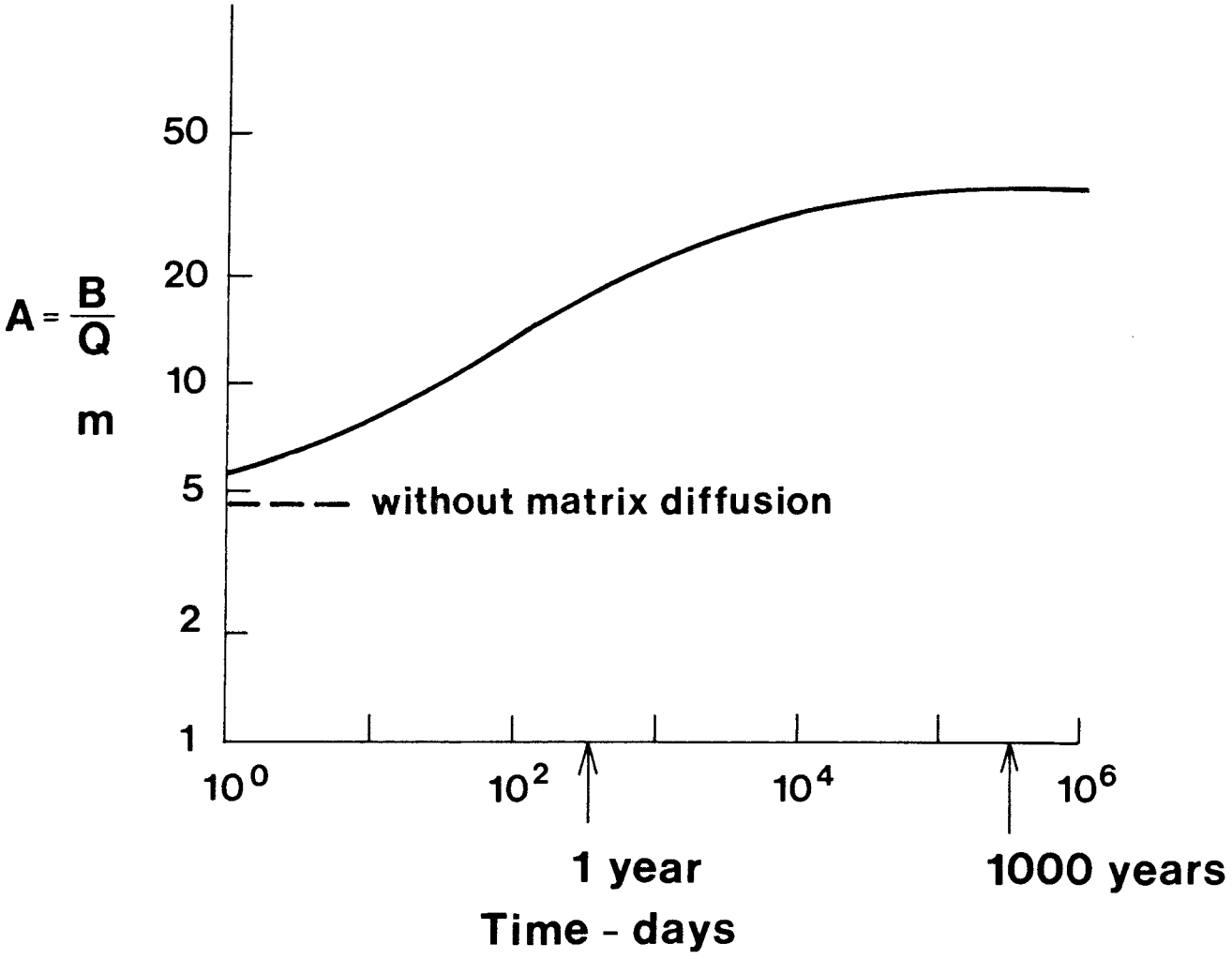

Figure 4 Fracture macrodispersivity with matrix diffusion; for λ = 1 m, D = 10^{-14} m^2/sec, n = 10^{-2}, σ_β^2 = 4, $\bar{b}$ = 100 μm.

that the results for variable surface sorption are analogous to similar results for the three-dimensional porous medium case (*Garabedian and Gelhar* (1985)).

The theoretical results developed here demonstrate how the large-scale dispersion process in a single fracture is influenced by the local variations of hydraulic properties as well as by sorption and matrix diffusion. The aperture variation produces a variation of flow velocity in the fracture which is manifest as a large scale dispersion effect. When the surface sorption coefficient varies it also affects the local advection velocity of a sorbing solute, and consequently an independent variation in sorption leads to an increased dispersion effect. When the variation of sorption is related to the hydraulic characteristics, it may increase or decrease the dispersion. Matrix diffusion, being analogous to a retardation effect, also has an influence on the large scale dispersion coefficient. In this analysis the interaction between an unsteady mean concentration field and the variation in storage due to aperture variation is a very important element. This interaction seems to be much more important in a fracture flow than in porous media where the analogous quantity would be a porosity variation.

The analysis developed here invoked a number of assumptions, a key one being that of relatively small perturbations. Previous experience with this approach (*Gelhar* (1986)) indicates that the perturbation approximation is valid for rather large variability, especially in the case of the flow equation. The theory should also be extended to treat a statistically anisotropic aperture process and transverse dispersion. In any case there is a need for careful numerical and field experimentation to evaluate the limitations of the theory presented here. Monte Carlo-type simulations for this two-dimensional system should be numerically quite feasible. Field experiments could be designed to test some of these results. The approach would be to measure the local variation of fracture aperture, transmissivity, surface sorption, and matrix diffusion. This local data could then be used to estimate the statistical parameters required to calculate the large-scale parameters from the stochastic theory. Then large-scale hydraulic and tracer tests would be carried out to determine the large-scale transmissivity, solute aperture and macrodispersivity. This approach then allows independent comparisons of the predictions from the stochastic theory with the large scale field observations and thereby avoids the usual curve-fitting approach.

When interpreting field observations of concentration in a variable aperture fracture it is important to recognize that the concentration represented by the theory is strictly a probability average or an ensemble mean. Evoking the ergodic

hypothesis, the mean concentration of the theory would be equivalent to a local areal average concentration. However, concentration measurements in the field more likely would involve a flow-weighted concentration. This difference can be accounted for as follows. The mean flow-weighted concentration is defined as

$$\tilde{c} = E[Q_1 c]/E(Q_1) \qquad (2.72)$$

$$= \bar{c} + \frac{E(Q_1' c')}{Q}$$

where the mean flow again is in the x_1 direction. The cross-correlation term in the second line of (2.72) is easily evaluated from the stochastic theory. Following the approach in (2.31) and (2.32), it is evident that

$$E(Q_1' c') = - \tilde{A} Q \frac{\partial \bar{c}}{\partial \xi_1} \qquad (2.73)$$

where $\tilde{A}$ is a modified dispersivity. Using this expression in (2.72) and substituting c from (2.72) it is easily shown that

$$b \frac{\partial \tilde{c}}{\partial t} + Q \frac{\partial \tilde{c}}{\partial x_1} - B \frac{\partial^2 \tilde{c}}{\partial x_1^2} = 0 \qquad (2.74)$$

where the result has been converted to the fixed coordinate system. This result shows that the same mean transport equation applies to the flow-weighted concentration. This shows that tracer tests in which flow-weighted concentration is measured can be interpreted using the usual advection dispersion equation, and that the same transport coefficients apply.

Applications of the results of the stochastic theory developed in this chapter could be of two types. First, the relationships for the hydraulic to solute aperture ratio and the macrodispersivity could be used in large-scale network models to portray more realistically the hydraulic and transport properties of individual fractures. This would be done simply by using a smaller hydraulic aperture to calculate the head drop in a fracture. The dispersion in an individual fracture would then be calculated from expressions such as (2.48) which predicts much higher dispersion than would be calculated from the classical

Taylor result. Secondly, the results here might be used directly to interpret the behavior of large−scale continuous fracture zones. In the next chapter some of the field information from existing experiments is reviewed as it relates to the stochastic theory.

3. ANALYSIS OF FIELD EXPERIMENTS

3.1 Purpose and scope

The primary goal of the analysis and interpretation developed here is to examine quantitative information from existing field experiments on solute transport in single fractures, emphasizing features relating to the stochastic theory developed in Chapter 2. This review focuses on several tracer experiments that have been carried out in Sweden, as well as one recently reported test in Canada. For each of the sites considered, the general description of the site and the actual test configuration were reviewed before proceeding with data analysis. Then an independent reanalysis of the hydraulic and tracer data was undertaken. Finally the revised parameters which resulted from the data analysis were interpreted in terms of the predictions from the stochastic theory. Some related laboratory and field experiments were also reviewed and those are discussed briefly.

3.2 Methods of interpretation

Here the general approach which was used to analyze the field data is outlined with emphasis on the convergent radial flow configuration employed in several of the tests. The configuration of the radial convergent tracer test system is illustrated in Figure 5. Hydraulic and tracer measurements in this configuration can be used to calculate large-scale fracture parameters. The tracer is introduced through the observation well at the radius r_2 from the pumping well with radius r_1. Assuming that the fracture behaves on a large scale as a homogeneous fracture, the transmissivitity of the fracture can be evaluated for steady flow as follows

$$T = \frac{q}{2\pi \Delta h} \ln (r_2/r_1) \qquad (3.1)$$

where q is the flow rate and Δh is the head drop between the observation and pumping wells.

The hydraulic aperture can then be calculated from this transmissivity using (2.17)

$$b_h = (12\nu T/g)^{1/2} \qquad (3.2)$$

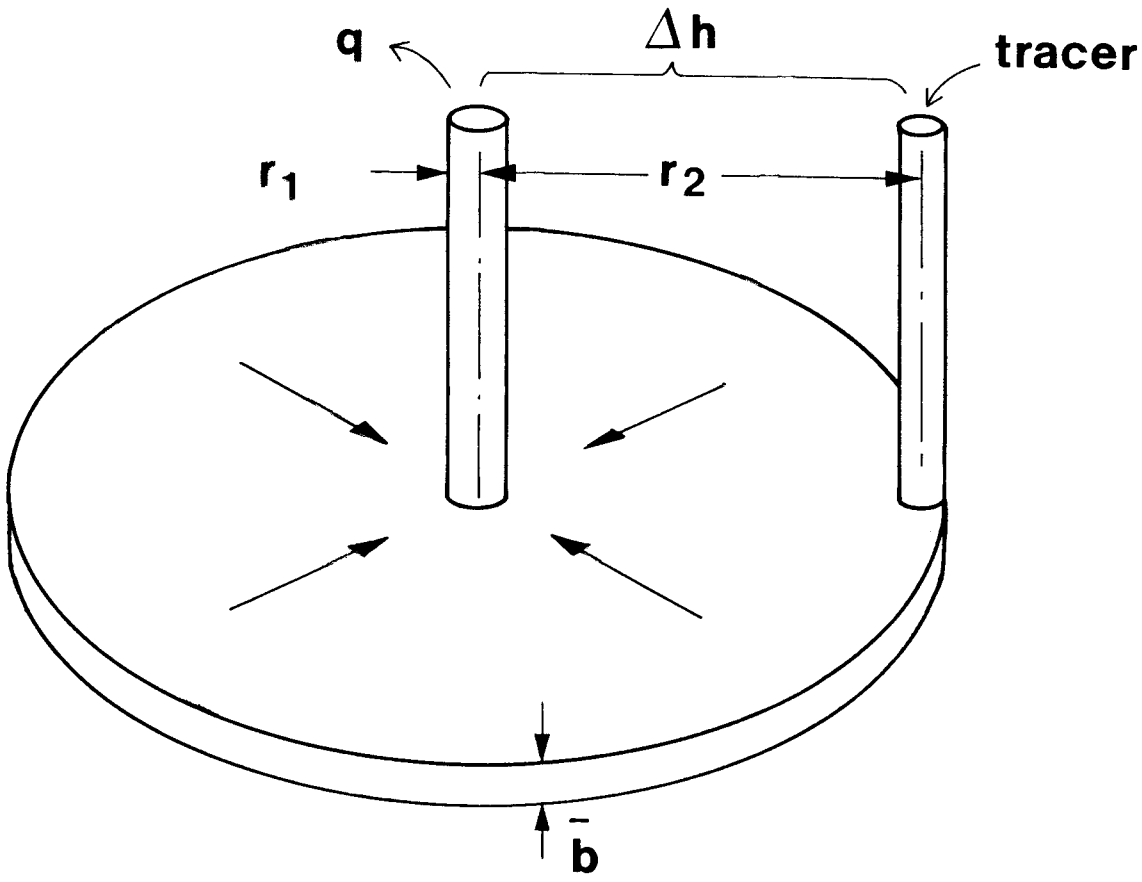

Figure 5 Convergent radial flow tracer test configuration.

The tracer tests consisted of either a pulse or a continuous injection of tracer at the observation well. The solute aperture of the fracture was determined from the mean residence time of the tracer t_0, the flow rate, and the volume of the fracture as follows

$$b_c = \bar{b} = qt_o/\pi(r_2^2 - r_1^2) \qquad (3.3)$$

The residence time and the dispersivity were estimated from the tracer breakthrough curves as depicted schematically in Figure 6. For the pulse input case the dispersivity was estimated from

$$A = \frac{3r_2}{64}\left[\frac{\delta t}{t_p}\right]^2 \qquad (3.4)$$

and for the step input case

$$A = \frac{3}{16\pi}\left[\frac{\Delta t}{t_{50}}\right]^2 \qquad (3.5)$$

These expressions are based on the general theory of *Gelhar and Collins* (1971) as applied by *Welty and Gelhar* (1986) to the convergent radial configuration. Those solutions take into account the varying velocity and dispersion coefficient associated with the radial flow system. These results are based on approximate solutions which are strictly valid for large Peclet number, say $r_2/A > 10$. These expressions are preferred over the more commonly used one−dimensional approximation (*Lenda and Zuber* (1970)), because they correctly account for the effect of the varying velocity. The one−dimensional expressions do not account for this varying velocity and consequently will overestimate the magnitude of the dispersivity by the factor 4/3. Consistent with the large Peclet number approximation, the time to peak for the pulse and the time to 50 % concentration for the step are used as the estimate of mean residence time of the solute.

Methods such as those outlined above were used where possible to develop independent estimates of the hydraulic and transport properties for each of the field sites.

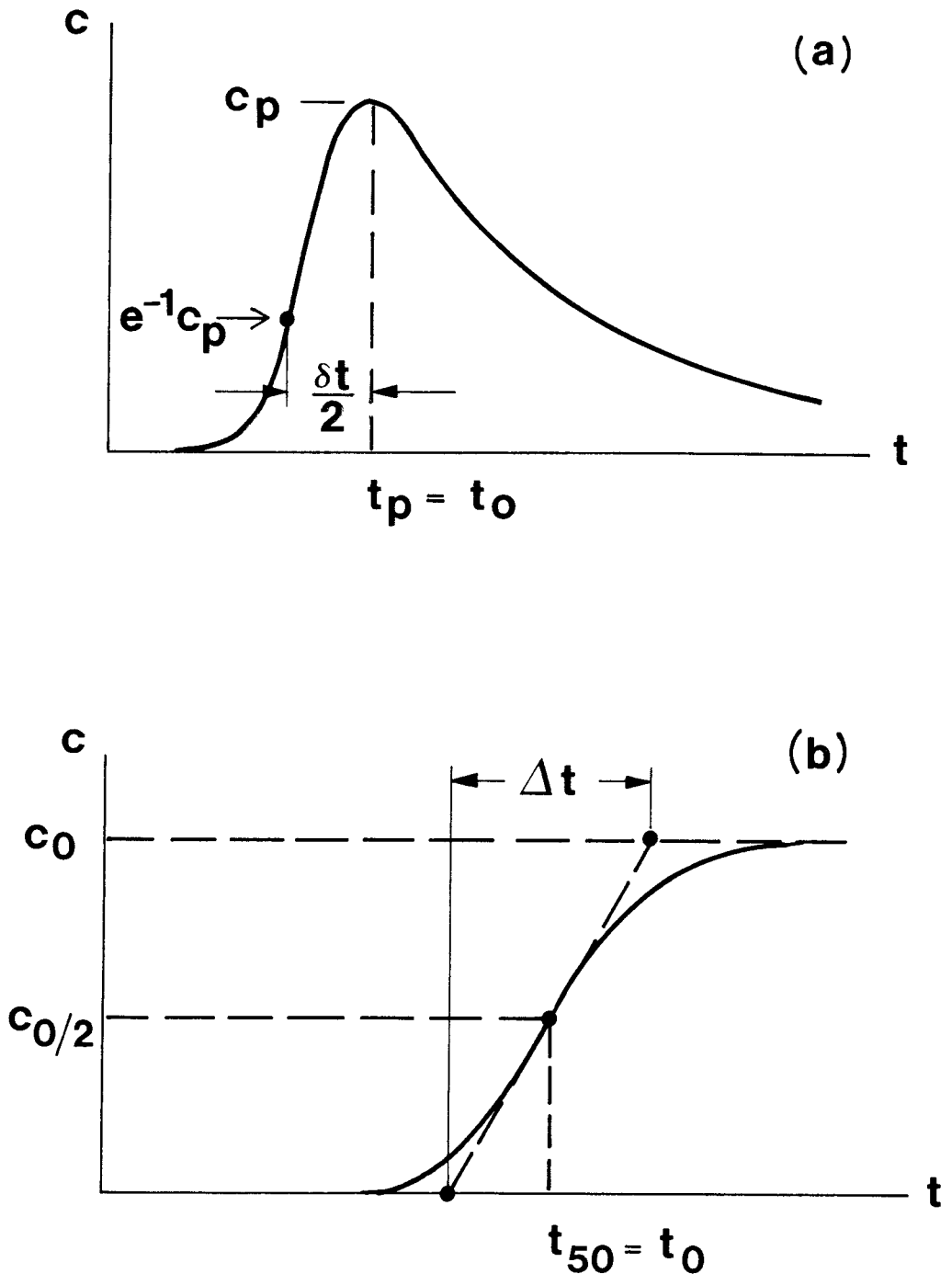

Figure 6 Schematic tracer breakthrough curves for convergent radial flow tracer tests; a) pulse input b) step input.

3.3 Interpretation for field sites

Data from four different field sites were analyzed to obtain estimates of hydraulic and transport parameters, and to infer stochastic parameters for the theory in Chapter 2. Some key features of each of the field experiments are discussed below. Table 1 summarizes some overall features of each experimental site. At each site, only the behavior of nonsorbing, nonreacting tracers was considered.

The field experiments at the Studsvik site are described by *Klockars and Person* (1982). Additional experiments with sorbing tracers at the Studsvik site are described by *Landström et al* (1983). *Klockars and Person* (1982) indicate that a zone consisting of several fractures was actually tested, but there is no explicit information on the individual fractures. Therefore it is not possible to make an independent calculation of the hydraulic properties. For this analysis, the hydraulic conductivity k_p given in Table 6.5D of *Klockars and Person* was used along with the thickness of the tested zone, 1.3 meters, to arrive at a transmissivity. Only test B involving the flow path B1N−B6N was analyzed. This path was supposed to have four fractures (*Klockars and Person* (1982), Table 3) each of which carried an equal amount of flow. From that hydraulic information, the hydraulic aperture in Table 1 was calculated. The tritium breakthrough curve, Figure 6.3C, was used to determine the residence time and dispersivity for this test. The solute aperture shown in Table 1 was calculated from the residence time and the flow for an individual fracture. The dispersivity given in Table 1 is somewhat lower than the value determined by *Klockars and Person*, probably because their one−dimensional analysis did not account for radial flow effects. The breakthrough curves for the tests at the Studsvik site all show very extensive tailing which, in my opinion, reflects the effects of unknown mixing conditions in the injection borehole and in the pumping borehole. The description of the experiment is not adequate to evaluate the nature of these effects, but it is my experience that for low porosity rocks such borehole effects can be dominant in the radial convergent flow system. For this reason only the rising part of the breakthrough curve was considered in the analysis.

The field experiment at the Finnsjön site is described primarily in *Gustafsson and Klockars* (1981). Additional pertinent information is found in *Gustafsson and Klockars* (1984). There the flow rate and the head drop are given and using

TABLE 1. Summary of data from tracer tests

Site	STUDSVIK	FINNSJÖN	STRIPA-2D	CHALK RIVER
test configuration	convergent radial pulse	convergent radial pulse	convergent radial ~ 1D step	doublet pulse
Displacement distance m	12	30	4	11
b_n μm	38	180	6.6	60
b_c μm	680	990	120	600
b_c/b_n	9.8	5.5	19	10
A m	0.3	1.0	0.9	1.4
σ^2_{lnb}	4.7	3.4	5.9	4.6
λ m	0.2	0.2	1.2	0.6

the packer test data from Figure 6.1A of *Gustafsson and Klockars* (1981), it was estimated that 31 % of the pumped flow was contributed from the tested zone.

Using this information the fracture transmissivity was determined and the hydraulic aperture shown in Table 1 was calculated. The breakthrough curves in Figures 6.21 A–B of *Gustafsson and Klockars* (1981) were used to estimate the mean residence time and the dispersivity. The resulting solute aperture and dispersivity are shown in Table 1. The dispersivity is somewhat lower than the value determined by *Gustafsson and Klockars* (1981). The breakthrough curves again show very extensive tailing which, in my opinion, is due primarily to borehole mixing effect. The information in the report is not adequate to evaluate this effects; therefore, the analysis was developed using only the rising part of the breakthrough curve.

Hodgkinson and Lever (1982) have also analyzed some of the tracer tests at the Finnsjön site. Their analysis included the effects of radial flow and of matrix diffusion, but assumed that the dispersion coefficient was proportional to the square of the velocity. Their analysis also incorporated a boundary condition which was intended to account for the effect of mixing in the pumping borehole. In my view their boundary condition is not physically realistic in that it imposes a uniform concentration throughout the length of the pumping borehole and in the fracture at the pumping well. Their analysis yields an equivalent dispersivity which is an order of magnitude lower than that determined here or estimated by *Gustafsson and Klockars* (1981), and they used a molecular diffusion parameter which was several orders of magnitude larger than values found from laboratory tests. Their analysis uses matrix diffusion simply as a curve–fitting device to represent tailing which is actually due to physical mixing conditions in the injection and pumping boreholes. *Moreno et al* (1983) have also analyzed tracer tests at the Finnsjön site using several different one–dimensional models. They have shown that the observed tailing can be fit adequately with several different models.

The data for the Stripa experiment are presented by *Abelin et al* (1985). The flow situation in this case was approximated as a radial flow through a 43 degree sector into the ceiling of the tunnel which was approximated as a circular arc. The total flow through this sector was measured to be 23 ml/hour (see their Figure 6.2) and the natural pressure gradient was determined from data given in Appendix A4. From this information the transmissivity was calculated

and the hydraulic aperture was then determined from (3.2). This steady-state transmissivity estimate is of the same order of magnitude as determined from the transient pressure tests. The tracer test information was from the second injection at H2 (Figures 6.6 and 6.7). The iodide breakthrough curves were used and it was assumed the breakthrough curves had reached the maximum concentration. The dispersivity and solute aperture were then calculated using the step input results for a one-dimensional flow to calculate the dispersivity. In this case the flow configuration is essentially one-dimensional because the displacement distance of four meters is small compared to the inner radius of approximately 15 meters. This experiment with separate sampling points along the intersection of the fracture with the ceiling of the tunnel is best analyzed in terms of the flux concentration, as discussed in Section 2.6. However, it was observed that iodide breakthrough curves at sampling holes 2.6 and 2.8 (Figures 6.6 and 6.7) are practically the same in shape, so that the calculation of a flow-weighted concentration is not necessary in this case.

The first injection at H2 was not analyzed because this test was very strongly influenced by the large initial injection rates, practically equal to the natural flow, and by the time-varying injection rate and resulting variable mass input of tracer. It is felt that this injection rate history is the dominant effect in determining the shape of the breakthrough curves in this case. *Abelin et al* (1985) have analyzed the first injection using several different one-dimensional curve-fitting models. I feel that their results demonstrate that the first injection is dominated by the time-variable tracer injection pattern. In some cases their dispersivities were of the same magnitude as was found here for injection 2 at H2.

The fourth site which was analyzed here is at Chalk River in Canada, as described by *Lever et al* (1985). This test differed from the previous three experiments in that it involved a doublet type flow configuration produced by a pumping-recharge well pair. In this case no hydraulic information was given other than a hydraulic aperture which the authors indicate was determined in earlier tests; that value is shown in Table 1. *Lever et al* (1985) analyzed the breakthrough curves from this test using an analytical solution for the one-dimensional constant coefficient advection-dispersion equation, applied to several stream tubes between the recharge and pumping wells. This approach was found to give an excellent fit of the breakthrough curve over the entire range of the experiment (see Figure 7). The breakthrough curves were also reanalyzed using the type curves developed by *Gelhar* (1982) which include the effect of

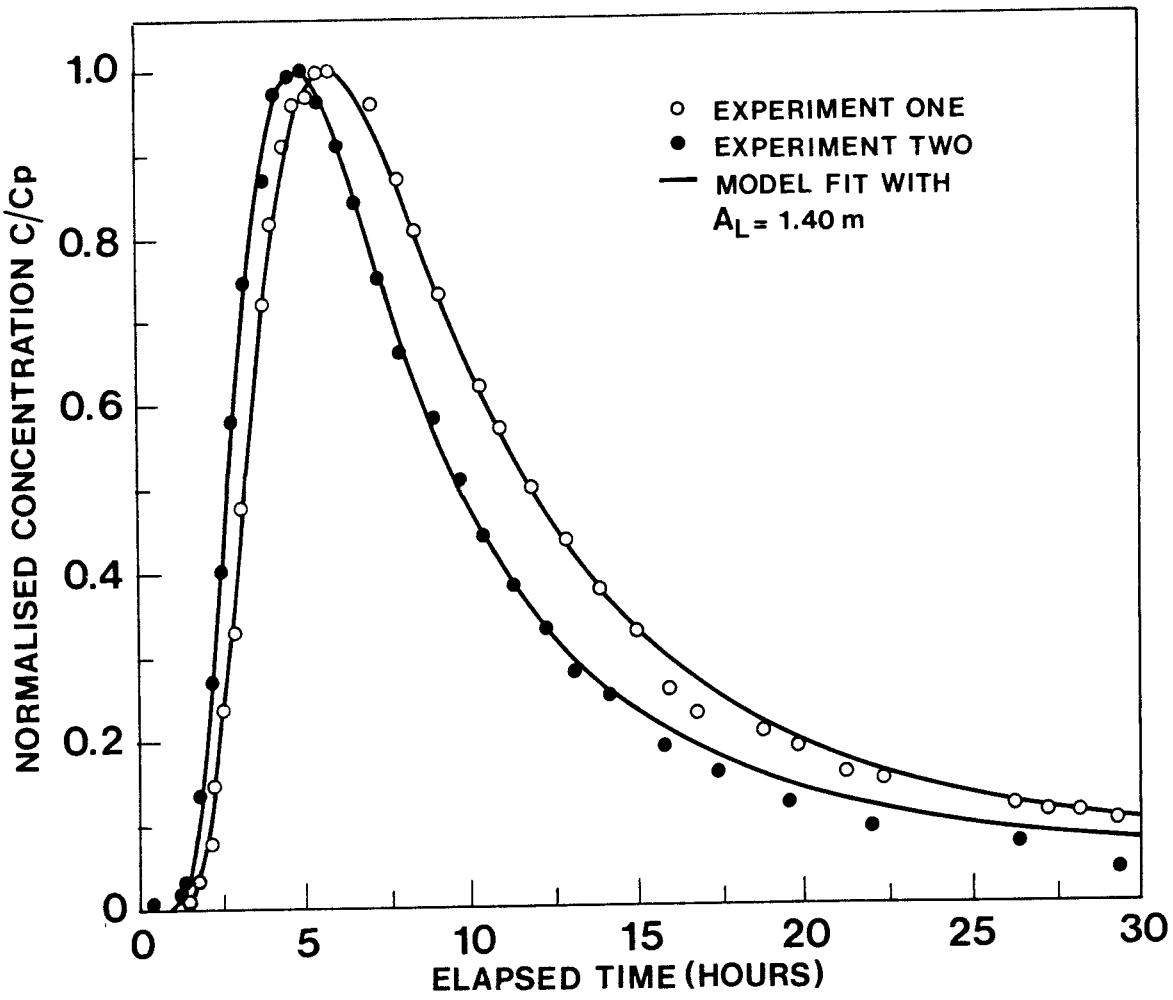

Figure 7 Comparison of advection−dispersion model with experiments for the doublet test at Chalk River.

the variable velocity field on the dispersion process. That model also fits the data very well and gives similar values for the solute aperture and the dispersivity; the only significant change was in b_c which is somewhat larger than 510 μm found by *Lever et al* (1985).

The data developed in Table 1 can be interpreted in terms of the results of the stochastic theory developed in Chapter 2. For the nonsorbing, nondiffusing case, the ratio of the hydraulic to the solute aperture is given by (2.49) from which the value of the variance of lnb can be calculated. These values are shown in Table 1 and are in the range of 3 to 6. Also, the dispersivity predicted by the stochastic theory (2.48) can then be used along with the calculated value of the variance of the logaperture to estimate the a value for correlation scale λ. These calculated values of the correlation scale are also shown in Table 1. These results indicate that the correlation scale is on the order of a meter or somewhat less. Values in this range are plausible and are consistent with the flow variations observed in the Stripa single fracture experiment (*Abelin et al* (1985)). Note that in the case of the Stripa site the calculated correlation scale is roughly one meter, whereas the overall scale experiment is only 4 meters. Under these conditions one cannot expect that the dispersivity has reached an asymptotic value and significant variations around the ensemble mean concentration would also be anticipated. In the other cases the correlation scale is at least an order of magnitude smaller than the displacement distance, so that the asymptopic ensemble mean theory should be a reasonable approximation. These calculations show that the stochastic theory can provide a consistent explanation of the dispersion process and of the difference between the solute and hydraulic apertures in a single fracture. These results, of course, do not prove that the proposed mechanism actually describes the dominant aspects of the fracture transport process. However, the results are encouraging enough to suggest that the theory should be evaluated more thoroughly through carefully designed experiments as discussed in Section 2.6.

3.4 Role of matrix diffusion

Matrix diffusion effects were not considered in any of the analyses summarized in Table 1. Based on a brief review of available laboratory and field information on matrix diffusion, it is felt that there is no definitive evidence that matrix diffusion is of any significance at the time scale of these tracer experiments. Furthermore, only the early rising limb of the breakthrough curves was analyzed,

this being the portion which is least affected by matrix diffusion. Of course, there is no question that the process of diffusion in a porous matrix exists. The key question is rather the magnitude of the effective diffusion coefficients under natural subsurface conditions. The extensive laboratory experiments reported by *Skagius* (1986) show a high degree of variability in the diffusion coefficient and significant effects of changes in mechanical stress. The field observations on an excavated fracture at Stripa (*Abelin et al* (1985)) also show extreme variability of apparent migration into the surface of the fracture. However, these field experiments are not definitive with regard to matrix diffusion because of the surface roughness of the natural fracture which makes it difficult to distinguish between surface sorption and migration into the rock matrix via diffusion. If depth profiling had been done for nonsorbing species, it may have been possible to resolve this question more definitely.

The field experiments of *Birgersson and Neretnieks* (1982, 1983) are often cited as evidence of matrix diffusion in the field. Of course, these experiments did not involve a natural fracture under natural flow conditions. This borehole test was done with the substantial overpressure which produced significant advection of solute into the rock matrix. This advection effect was considered in the analysis of the data, but the mechanical dispersion that would be produced by such a flow was neglected. Some rough calculations of the mechanical dispersion effect in this experiment indicate that much of the observed spreading could be explained as mechanical dispersion rather than diffusion.

Then, of course, there are the numerous tracer tests that have been analyzed by fitting matrix diffusion models to represent the extended tails frequently observed with radial convergent tests. It is more likely that these tailing effects are produced as a result of complicated mixing processes in the injection or pumping boreholes, or because the dispersion process has not developed to its asymptotic limit. *Welty and Gelhar* (1986) have developed solutions which demonstrate the strong effect of borehole flushing and placement−dependent dispersion in the radial convergent configuration. Several radial convergent tracer tests were reinterpreted in that report. Even in high porosity granular porous media where matrix diffusion would not be as significant, very extensive tailing is commonly observed.

It is safe to say that the role of matrix diffusion under actual field conditions in fractured crystalline rock remains unresolved. The stochastic theory developed in Chapter 2 does provide a systematic framework for looking at the interaction

between the channeling process associated with the variable aperture fracture and the matrix diffusion process. The results developed there (Figure 4) suggest that matrix diffusion can have significant effects at large times. The resulting increased dispersion may negate some of the retardation effects of matrix diffusion and lead to an earlier arrival of contaminants at a point of discharge. In any case there is clearly a need for carefully designed field experiments which can definitively evaluate the significance of matrix diffusion.

3.5 Potential applications of three-dimensional stochastic theory

The theoretical approach developed in Chapter 2 emphasizes the behavior of a single fracture, and therefore is applicable at relatively small scales, say at most tens of meters. The approach might also be applicable to large-scale fracture zones in otherwise sound rock. However, for extensively fractured systems it seems that a three-dimensional treatment will be necessary in order to describe the large-scale behavior on scales of hundreds or thousands of meters. The continuum stochastic theory developed by *Gelhar and Axness* (1983) can in principle describe the dispersion process in heterogeneous, statistically anisotropic porous medium continuum. In view of the very extensive fracturing that seems to be observed in the rocks in Sweden, it may be possible to use a theory of this type to treat the large-scale transport process in these fractured rocks. In fact, data from large-scale tracer tests in porous and fractured media (*Gelhar et al* (1985)) do not show any significant difference between dispersivities in porous media and dispersivity at the same scale in fractured media. This information is summarized graphically in Figure 8. What is required in order to apply the theory of *Gelhar and Axness* is measurements of the variability of hydraulic conductivity in three dimensions. These data are then used to estimate the three-dimensional covariance function of log hydraulic conductivity which is required to predict the macrodispersivity tensor. The variation in hydraulic conductivity can be determined from short interval packer tests in boreholes. *Winter et al* (1985) have discussed the application of this approach to fractured rock at the Oracle site in Arizona, although they considered only the isotropic case.

Large-scale hydraulic testing can also be used to infer some of the parameters required for three-dimensional stochastic theory because the large-scale hydraulic anisotropy is dependent on the statistical anisotropy of the log hydraulic

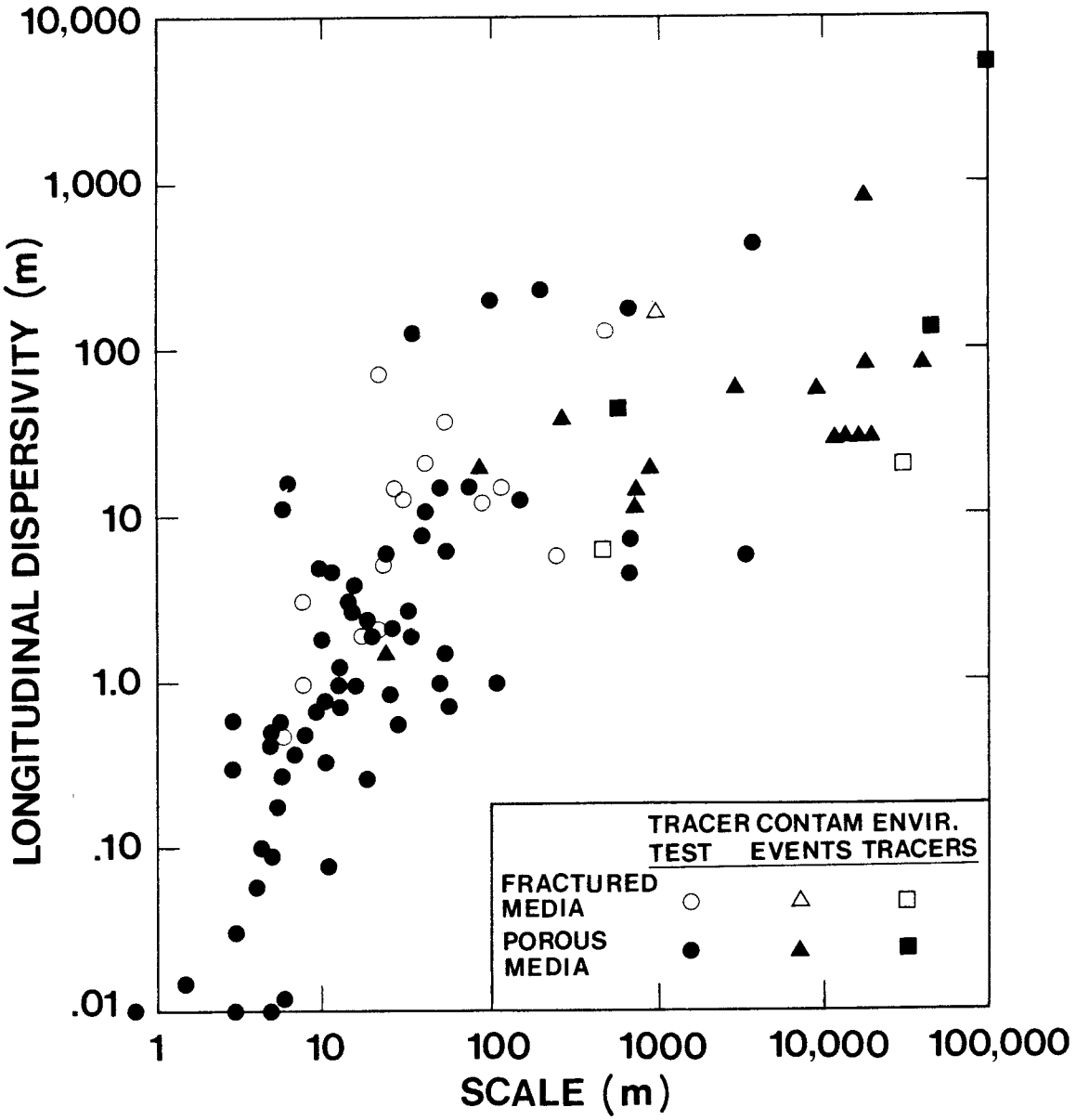

Figure 8 Field scale longitudinal dispersivities for porous and fractured media.

conductivity covariance function. This approach has been persued by *Hufschmied* (1985) for a gravel aquifer in Switzerland.

The Finnsjön site (*Carlsson et al* (1983), *Ahlbom et al* (1986)) would seem to be a good prospect for application of the three-dimensional stochastic transport theory. There are number of existing boreholes at that site which could be tested and used for large-scale hydraulic tests. The angled boreholes have the unique advantage that they make it possible to determine the three-dimensional anisotropy of the log hydraulic conductivity covariance function. Packer spacings as small as possible, say down to a meter, would be required in order to resolve the correlation scales anticipated in the covariance function. Around a hundred sampling points would be required in each borehole to develop a satisfactory estimate of the covariance function. The large-scale hydraulic tests could be designed and interpreted following the approach of *Hsieh et al* (1983) to determine the three-dimensional hydraulic anisotropy. This same kind of large-scale hydraulic testing configuration could be used to develop large-scale tracer tests for the site which could then form the basis for an evaulation of the prediction from the three-dimensional stochastic theory.

In order to treat the case of sorbing and diffusing solute it will be necessary to generalize the three-dimensional stochastic theory to include a source-sink term associated with the sorbing or diffusing surface area per unit volume in the fracture medium.

3.6 Recommendations for field experiments

Experiments at several scales will be required in order to resolve the nature of the transport process in fractured rocks. The theory developed in Chapter 2 provides a specific predictive hypothesis which can be tested in small-scale field experiments on individual fractures. Within a single fracture measurements of the local variation of hydraulic properties of the fracture could be made using small scale packer tests, as proposed by *Neretnieks* (1986) for the Stripa phase III investigations. Observations of the variation in fracture aperture would also be needed in order to apply the stochastic theory, and if sorption and diffusion are considered, measurements of the spatial variability of these properties on the surface of the fracture would also be needed. Covariance or variogram analysis can then be applied to the spatial data to estimate the pertinent covariance scales and develop an independent prediction of the transport properties.

In view of the consistently troublesome behavior of the convergent radial flow tracer test, especially in low porosity rocks, it is strongly recommened that the two-well doublet configuration with a pulse input of tracer also be considered for tracer tests. It is my experience that this test is much less sensitive to borehole storage and mixing effects than the radial convergent test which in some way depends on ambient flow to remove the tracer from the injection borehole. The experience with the doublet test has been quite favourable in that it lends itself to simple interpretation with a minimum number of adjustable parameters, as discussed with reference to Chalk River site in Section 3.3. A type curve for the doublet configuration with nonreactive solute is shown in Figure 9. From this figure it can be seen that dispersion has a strong influence on the rising and peak part of the breakthrough curve, but that the tail is essentially determined by the large-scale advection pattern of the doublet. Therefore the characteristics of the matrix diffusion model as discussed in Section 2.5 suggest that the doublet test can be used to advantage to look for the effects of matrix diffusion. The short direct flow paths which affect the dispersion process will not be influenced by matrix diffusion but, considering that there is a time-varying retardation effect associated with matrix diffusion, one would expect that the shape of the advection-determined tail of the breakthrough curves would be significantly affected. In a sense the wide variation in travel time which is associated with the doublet configuration could be used to advantage to try to sense matrix diffusion effects. Of course, efforts to use tracers with significantly different molecular diffusion coefficients should also be continued.

Large-scale hydraulic and tracer tests are also suggested along the lines of the discussion in the previous section. In spite of what calculations from matrix diffusion models might suggest, I believe it is feasible to carry out a tracer test in fractured crystalline rock over scales of several hundred meters, especially since this has been done at the Savannah River site for a doublet-type test with a well spacing of over 500 meters (*Webster et al* (1970)). If clearly defined fracture zones can be identified from hydraulic testing, a two-dimensional doublet configuration would be appropriate. If the hydraulic behaviour seems to be fully three-dimensional, it may be necessary to develop a three-dimensional doublet test and type curves similar to those in Figure 9 for that situation. Of course, here I am suggesting borehole testing from the surface. Finnsjön site seem to be a good prospect for this kind of investigation.

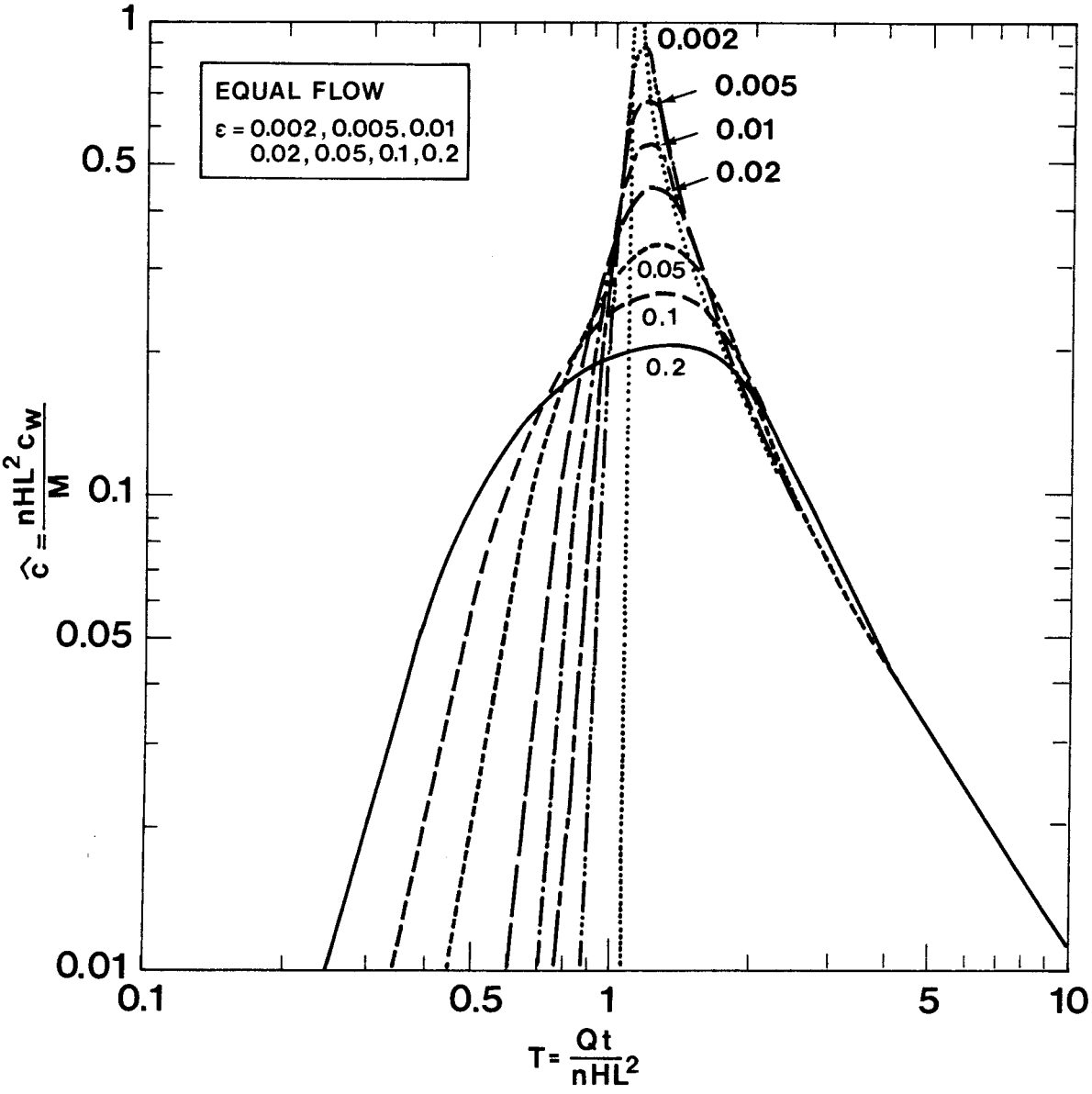

Figure 9 Type curve for the two−dimensional pulse input doublet tracer test; ϵ = α/L, α = longitudinal dispersivity, L = well spacing, Q = pumping rate, n = porosity, H = aquifer thickness, M = mass of tracer injected, c_w = concentration in pumping well, t = time (from *Gelhar* (1982)).

At intermediate scales, say of the order of a hundred meters, a three-dimensional doublet configuration may be useful for tracer tests executed from boreholes drilled outward from a mine drift at Stripa. In this way one could get away from the flow influence of the mine. Using several holes at different angles, it should be possible to investigate the dependence of the large-scale transport properties on the scale of the experiment.

4. CONCLUSIONS AND RECOMMENDATIONS

4.1 Conclusions

Important overall conclusions which have evolved from this work include:

1) The stochastic theory for flow in a single variable aperture fracture provides a unified description of the key transport features of a natural heterogeneous fracture, i.e., the channeling effect as reflected in the difference between the solute−based and hydraulically−based apertures, and the macrodispersion produced as a result of the spatially−variable velocity field in fractures.

2) The stochastic theory predicts that the surface sorption and matrix diffusion can have a significant effect on the macrodisperison process in a single fracture, increasing the dispersivity for sorbed or diffusing solutes as much as an order of magnitude over those for nonsorbing, nondiffusing solutes.

3) A reexamination of the results of tracer tests on individual fractures at four different sites shows features which are consistent with the predictions of the stochastic theory. Correlation scales for the logaperture variation are calculated to be on the order of a meter.

4.2 Recommendations

Based on results and experience from this study, it is suggested that the following be investigated in future work:

1) The stochastic theory developed here involves a number of simplifying assumptions and approximations which need to be evaluated. These points are discussed in detail in Section 2.6, but of particular concern is the small perturbation approximation which is used in developing the analytical solution. Carefully designed numerical experimentation is required to evaluate the importance of that approximation.

2) The stochastic theory should be extended to more general situations involving variable matrix diffusion, statistical anisotropy of aperture variability and transverse dispersion.

3) The stochastic theories described in this report provide a specific framework for predicting large-scale transport properties of fractured rocks. The theory has the feature that it can use small-scale measurements of the heterogeneity of various parameters in order to predict the large-scale behavior. In this sense the stochastic theory provides a hypothesis which can be subjected to independent field evaluation. A number of field experiments along these lines have been suggested in detail in Section 3.7. These should include experiments at a small scale, on the order of ten meters, focusing on individual fracture behavior, as well as very large scale experiments up to a kilometer in extent which can be related to continuum stochastic theories.

4) This final recommendation has more to do with the administrative aspects of large field testing programs of the type that have been going on in Sweden. These are scientifically unique and significant experiments, but my experience has been that the documentation of the experimental work is in many cases not adequate. The data are often presented in an incomplete form which emphasizes only that information needed for the interpretations presented in that report. Because of the inadequate documentation much of the scientific value of these unique experiments may be lost. I therefore strongly recommend that strict standards be established for documentation of field experiments, and that financial resources be made available for preparation of proper documentation. Anonymous peer reviewing may also be appropriate for the reports. Basic data reports which are separate from interpretation and analysis may also be appropriate. Some very unique, complicated and expensive experiments have been proposed for crystalline rock in Sweden. In order to obtain optimal scientific benefit from these unique experiments I feel it would be wise to establish a formal review process with outside independent experts who will review and comment on proposed experimental designs.

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Division of Rock Mechanics,
Luleå University of Technology, Sweden
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Department of Neclear Chemistry, Chalmers University of Technology, Göteborg
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Department of water in environment and society, Linköping university, Linköping
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Mikael Sehlstedt, Swedish Geological Co, Malå
Erik Gustafsson, Kenth Hansson, Olle Olsson,
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Göran Nilsson, Swedish Geological Co, Luleå
Karin Axelsen, Peter Wikberg, Royal Institute of Technology, Stocholm
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Swedish Geological Co, Uppsala
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Radar measurements performed at the Klipperås study site
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Fuel rod D07/B15 from Ringhals 2 PWR: Source material for corrosion/leach tests in groundwater
Fuel rod/pellet characterization program part one

Roy Forsyth
Studsvik Energiteknik AB, Nyköping
March 1987

TR 87-03

Calculations on HYDROCOIN level 1 using the GWHRT flow model
Case 1 Transient flow of water from a borehole penetrating a confined aquifer
Case 3 Saturated-unsaturated flow through a layered sequence of sedimentary rocks
Case 4 Transient thermal convection in a saturated medium

Roger Thunvik, Royal Institute of Technology, Stockholm
March 1987

TR 87-04

Calculations on HYDROCOIN level 2, case 1 using the GWHRT flow model

THERMAL CONVECTION AND CONDUCTION AROUND A FIELD HEAT TRANSFER EXPERIMENT

Roger Thunvik
Royal Institute of Technology, Stockholm
March 1987