Solute transport in a single fracture with negligible matrix permeability: 2. mathematical formalism

J. Bodin · F. Delay · G. de Marsily

Abstract This report provides an overview of the mathematical expressions for modeling fundamental solute transport mechanisms at the fracture scale. It focuses on low-permeability rocks where advection in the matrix is negligible as compared to that in fractures. The following processes are considered: (1) advective transport in fractures, (2) hydrodynamic dispersion along the fracture axis, (3) molecular diffusion from the fracture to the porous matrix, (4) sorption reactions on the fracture walls and within the matrix, and (5) decay reactions. The aim of this review is to gather in a single article the transport equations and their analytical solutions, using a homogeneous notation to facilitate comparison and exploitation.

Résumé Ce rapport présente une vue d'ensemble des expressions mathématiques proposées dans la littérature pour modéliser le transport de soluté à l'échelle de la fracture. L'accent est mis sur les roches faiblement perméables où le transport par convection dans la matrice rocheuse peut être considéré comme négligeable devant le transport dans les fractures. Les processus considérés sont les suivants: (1) transport par convection dans les fractures, (2) dispersion hydrodynamique, (3) échanges de soluté par diffusion moléculaire entre les fractures et la matrice rocheuse, (4) réactions de sorption sur les parois des fractures et à l'intérieur de la matrice et (5) réactions de décroissance. L'objectif premier de cette revue est de rassembler les équations de transport et leurs solutions analytiques en utilisant une notation homogène pour faciliter leur utilisation et les comparaisons.

Resumen Este informe proporciona una revisión de las expresiones matemáticas para modelar los mecanismos fundamentales de transporte de solutos a escala de fracturas. Se centra en rocas de baja permeabilidad donde la advección en la matriz es despreciable en comparación con la de las fracturas. Se considera los procesos siguientes: (1) transporte advectivo en las fracturas; (2) dispersión hidrodinámica a lo largo del eje de la fractura; (3) difusión molecular desde la fractura a la matriz porosa; (4) reacciones de sorción en la pared de la fractura y en la matriz; y (5) reacciones de degradación. El propósito de esta revisión es reunir en un único artículo las ecuaciones de transporte y sus soluciones analíticas con una notación homogénea para facilitar su comparación y aplicación.

Keywords Fractured rocks · Mathematical formalism · Solute transport · Topical review

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Introduction

Article 1 (Bodin et al. 2003) focused on the principal mechanisms that govern solute transport in a fracture: advection and hydrodynamic dispersion, channeling effects, matrix diffusion, and sorption reactions. This second article is intended to provide an overview of the mathematical expressions of the mechanisms cited above and to introduce them into the transport equations.

From a conceptual point of view, mathematical modeling of transport in fractured rocks is developed by following either a continuous or a discrete approach. In the continuous framework, the fractured system is represented by a unique continuum or by a series of continua. The details of the network geometry are overlooked, only the average properties of the fracture network and the rock matrix are considered. On the other hand, the discrete framework is based on the explicit representation of fractures and on the resolution of transport equations within each fracture.

Historically, the continuous approach has been the first one used for modeling flow and transport in fractured media. The idea was to refer to methods already available

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for porous media while replacing the real fractured system by an equivalent porous medium (EPM). Key parameters are the equivalent permeability and dispersion tensors. In a new approach to characterize heterogeneity, Tsang et al. (1996) developed a stochastic continuum model of fractured rock. The fractured areas are distinguished from the matrix by giving them high hydraulic conductivity values with long-range correlation. In parallel to single-continuum EPM modeling, some authors have developed another continuous approach based on two continuums to better distinguish the roles of fractures and matrix. The dual-media approach consists in associating a continuous medium to the matrix and a second one to fractures. The fluid and mass transfers between fractures and the matrix are conceived as exchange fluxes between both continuous media.

This dual-media approach was first developed by Barenblatt et al. (1960) and Warren and Root (1963) to solve flow problems in fractured porous rocks and was later used for transport models (Bibby 1981; Huyakorn et al. 1983a, 1983b; Gerke and van Genuchten 1996; Leo and Booker 1996; Arnold et al. 2000; Lichtner 2000). Transport equations are written for each medium considering advection–dispersion in fractures and diffusion in the matrix. Both equations are connected by a sink-source term to account for the exchanges between fractures and the matrix (Huyakorn et al. 1983a; Gerke and van Genuchten 1996).

The literature proposes various comments about the validity of continuous approaches (Long et al. 1982; McKay et al. 1993; Berkowitz et al. 1988; Guérin and Billaux 1994; Pankow et al. 1986; Sudicky and McLaren 1992). In summary, the continuous approach should be theoretically valid only if an elementary representative volume (ERV) exists, i.e., a volume of very small size as compared to the scale of the problem and in which flow and transport properties are statistically homogeneous. In practice, the concept of ERV is the most constraining one to justify the continuous approach because numerous studies have shown that natural fracture networks often exhibit multiscale or fractal organizations. In that case, the homogenization scale of the network is hard, or perhaps even impossible, to identify. Some authors challenge the existence of an ERV in fractured media and reject the continuous approach in favor of the discrete modeling.

In fact, the discrete approach may appear more intuitive and logical than the continuous one because transport mechanisms in each fracture are explicitly taken into account. Modeling, therefore, is viewed with less "non-physical" abstraction of the medium. The principal drawbacks of discrete models are the computational efforts and the parameterization. The discrete simulation of transport at the field scale (with thousands of fractures) implies much more difficult calculations than with the continuous approach. The number of required parameters is also larger; a priori the rigorous discrete approach requires one set of parameters for each element discretizing the fractures. Moreover, transport equations must be solved for each element, which demand large memory capacities of computers. In 1988, Berkowitz et al. expressed doubts about the possible use of discrete calculations for transport scenarios in a fractured reservoir of average extent. This was justified 15 years ago, but, today, the power and the memory capacity of computers double each year. This very rapid evolution makes one believe that discrete models will become handy tools for solving transport problems in fractured media. However, the question of parameterization still remains unresolved and all the more crucial since numerical simulations are conditioned on available data (see e.g., Smith et al. 1997).

Recently, the Swedish Nuclear Fuel and Waste Management Company (SKB) has conducted a comparative analysis of different modeling approaches to flow and advective transport in an hypothetical underground repository site in Äspö. For this study, also called Alternative Models Project (AMP), three modeling approaches were considered: stochastic continuum (Widén and Walker 1999), discrete fracture network (Dershowitz et al. 1999) and channel network (Gylling et al. 1999). The same reference problem was considered by the three approaches. The main results of this study are summarized by Selroos et al. (2002). The three modeling approaches predicted similar minimum- and median-travel times, and similar locations for pollutant outlets in the geosphere. This consistency suggests that the conceptual differences in the modeling approaches do not yield very different results provided they apply to a problem with the same well-defined settings.

The purpose of this report is limited to the mathematical formalism of transport in the discrete-fracture approach. The typical scale is that of the single fracture because the resolution of transport within each fracture plane and of mass sharing at fracture intersections enable one to model the behavior of a network. In the sequel, fractures are supposed to be rigid and empty, i.e., the matrix does not deform during the flow, and alteration byproducts or solid particles are unable to seal the fracture aperture. It must be noted, however, that the presence of fracture infilling may significantly alter the flow regime (Wealthall et al. 2001), the fractures acting sometimes as impervious barriers when filled with fine-grained, low-permeability sediment. At the kilometer scale, tectonic faults may also induce compartmentalized flow and transport if their throw breaks apart the connectivity of the lower-scale fractures (Bruel et al. 1999).

The physical mechanisms that play a part in transport in the fracture and the neighboring matrix (cf. article 1) are mathematically described and inserted into various transport equations. The aim is to gather in a single article the transport equations and their analytical solutions, using a homogeneous notation to facilitate comparison and exploitation.

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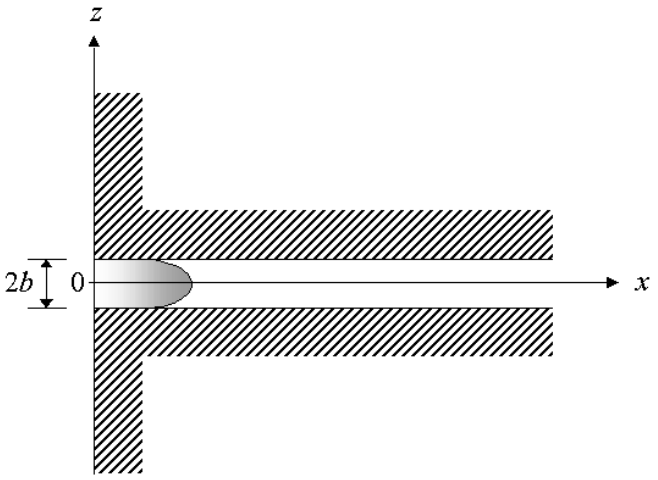

Fig. 1 Schematic illustration of solute transport in a single fracture without matrix diffusion

Advection–Dispersion in a Single Fracture

The simplest transport problem is the motion of a non-reactive solute in a single fracture with parallel and impervious walls. Even if this assumption is not appropriate with regard to natural fracture geometries, it remains, however, the basics of many complicated modeling approaches for flow and transport at the local scale. The conceptual model corresponding to the parallel-plate system is illustrated in Fig. 1. In that case, the principal transport mechanisms are advection and hydrodynamic dispersion. If the Fickian regime of dispersion is reached, and if transverse dispersion is neglected as compared to longitudinal dispersion, the volume concentration of solute in the fracture obeys the classical 1-D advection–dispersion equation in a homogeneous medium:

$$\frac{\partial c_f}{\partial t} = D_L \frac{\partial^2 c_f}{\partial x^2} - u \frac{\partial c_f}{\partial x} \tag{1}$$

with c_f $[M{\cdot}L^{-3}]$ the volume concentration of solute in the fracture; t $[T]$ the time variable; x $[L]$ the space coordinate along the flow direction in the fracture plane; u $[L{\cdot}T^{-1}]$ the mean fluid velocity in the fracture; and D_L $[L^2{\cdot}T^{-1}]$ the hydrodynamic dispersion coefficient in the fracture. D_L is generally given by the following expression (Tang et al. 1981):

$$D_L = \alpha_L u + D_m \tag{2}$$

where α_L $[L]$ is the dispersivity and D_m $[L^2{\cdot}T^{-1}]$ is the molecular diffusion coefficient of the solute in the fluid.

Given the nature of advection and hydrodynamic dispersion, the solute motion is controlled by the fluid velocity. Therefore, modeling the solute transport necessitates a precise characterization of flow in the fracture.

Flow Regime

As shown experimentally by Louis (1974), flow in a fracture of constant aperture $2b$ and roughness ε is laminar or turbulent according to the Reynolds number:

$$Re = \frac{2bu}{\upsilon} \tag{3}$$

and to the relative roughness:

$$Rr = \frac{\varepsilon}{D_h} \tag{4}$$

with $2b$ $[L]$ the fracture aperture; u $[L{\cdot}T^{-1}]$ the mean fluid velocity; υ $[L^2{\cdot}T^{-1}]$ the kinematic viscosity; ε $[L]$ the mean height of the fracture asperity; and D_h $[L]$ the hydraulic diameter defined as:

$$D_h = 4\frac{S}{P_{ext}} \tag{5}$$

where S $[L^2]$ is the flow section of the fracture and P_{ext} $[L]$ is the external perimeter of the flow section.

For a relative roughness $Rr \leq 0.033$, the transition from laminar toward turbulent flow is reached for $Re > 2{,}300$. When Rr is over the critical threshold of 0.033, the transition is reached for Reynolds numbers much lower than 2,300. According to Louis (1974), this limit decreases down to values of about $Re = 100$ for $Rr = 1$. Natural fractures often show rough walls with partial contacts between them. Their relative roughness is close to 1 and it is not surprising to observe divergences from Darcy's law when pumping tests are performed even with Reynolds numbers lower than 300 (Kohl et al. 1997). In the same way, Kosakowski and Berkowitz (1999) showed that "parallel plate" fractures might be subjected to turbulent flow at their intersections for Reynolds numbers of about 100. Thus, a 2-D description of flow at the intersections would be strictly valid only for $Re < 10$. However, in a reservoir under natural hydraulic-head gradient, flow can be considered as laminar. The apertures of natural fractures are mostly in the range 10 to 500 μm and, for a mean gradient of 10^{-3}–10^{-4}, the Reynolds number varies from 10^{-4}–1. This is different with pumping tests for which the forced flow is able to result in much higher values (Re up to 100, see Kohl et al. 1997).

Local Equation for Flow of an Incompressible Fluid

The fundamental Navier–Stokes equation for an incompressible Newtonian fluid in isothermal flow is:

$$\rho\left(\frac{\partial u_i}{\partial t} + \sum_{\lambda=x,y,z} u_\lambda \frac{\partial u_i}{\partial \lambda}\right) = \mu \sum_{\lambda=x,y,z} \frac{\partial^2 u_i}{\partial \lambda} - \frac{\partial P}{\partial i} + \rho g_i \tag{6}$$

where i=x, y, z; ρ $[M{\cdot}L^{-3}]$ is the mass density of the fluid; u_i $[L{\cdot}T^{-1}]$ is the scalar component of the fluid-velocity vector along the i direction; μ $[M{\cdot}L^{-1}{\cdot}T^{-1}]$ is the dynamic viscosity; P $[M{\cdot}L^{-1}{\cdot}T^{2}]$ is the fluid pressure; and g_i $[L^2{\cdot}T^{-1}]$ is the scalar component of the gravitational-acceleration vector along the i direction.

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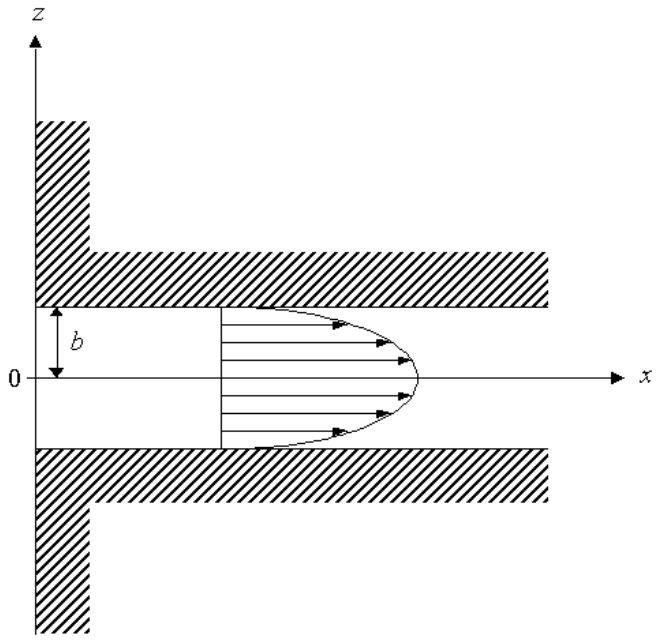

Fig. 2 Parabolic profile of fluid velocities for laminar flow between two smooth parallel plates

For steady-state flow, the inertial term (left-hand side) cancels out and the Eq. (6) becomes:

$$\mu \sum_{\lambda=x,y,z} \frac{\partial^2 u_i}{\partial \lambda} - \frac{\partial P}{\partial i} + \rho g_i = 0 \tag{7}$$

where $i=x,y,z$, which is also called the Stokes' equation. Solving the Stokes' equation in a parallel-plate system yields a parabolic profile of the fluid velocity along the flow section (Poiseuille's flow), as it is illustrated in Fig. 2:

$$u(z) = -\frac{b^2}{2\mu}\frac{dP}{dx}\left[1 - \frac{z^2}{b^2}\right] \tag{8}$$

where b [L] is the half-aperture of the parallel plates.

The flow rate per width unit is calculated by integration of the Eq. (8) over the aperture and is written:

$$Q_{funit} = \int_{-b}^{b} u(z)dz = -\frac{2b^3}{3\mu}\frac{dP}{dx} \tag{9}$$

(also referred to as the "cubic" law). Thus, the total flow rate is:

$$Q_f = -\frac{2}{3\mu}b^3 W\frac{dP}{dx} = -\frac{2\rho g}{3\mu}b^3 W\frac{\Delta H}{\Delta x} \tag{10}$$

with W [L] the width of the plates in the direction perpendicular to the pressure gradient; and ΔH [L] the variation of hydraulic head over the lag distance Δx.

By analogy with Darcy's law, the local hydraulic conductivity of a fracture with a local aperture $2b$ is defined as (Snow 1969; Bear 1993):

$$K_f = \frac{\rho g b^2}{3\mu} \tag{11}$$

Taking into account the roughness of walls, Louis (1974) proposes an empirical formulation of the hydraulic conductivity which is written:

$$K_f = \frac{\rho g b^2}{3\mu(1 + 8.8Rr^{1.5})} \tag{12}$$

Therefore, the mean fluid velocity in a fracture of aperture $2b$ follows the expression:

$$u = -K_f\frac{dH}{dx} = -\frac{b^2}{3\mu}\frac{dP}{dx} \tag{13a}$$

which allows one to rewrite Eq. (8) as:

$$u(z) = \frac{3}{2}u\left[1 - \frac{z^2}{b^2}\right] \tag{13b}$$

Contrary to porous media, the Darcy velocity in a parallel-plate system corresponds to the real mean fluid velocity since the fracture porosity is one. For rough walls with partial contacts between them, some authors attribute to the fracture a porosity less than one (Odling and Roden 1997). The equations mentioned above are basically written assuming that the walls are impervious, or of very low permeability. In other words, the drainage towards the matrix is negligible. For fractures with pervious walls, one may refer to Bear (1993). Kessler and Hunt (1994) also derived analytical expressions for the water velocities in a single fracture with porous material attached to the fracture walls. The influence of stress on fracture permeability is addressed by Adler and Thovert (1999), Gentier et al. (2000) and Mourzenko et al. (1997).

Laminar Flow in a Fracture with Varying Aperture

The geometric analysis of natural fractures shows that apertures may vary over narrow to wide ranges (Johns et al. 1993; Persoff and Pruess 1995; Hakami and Larsson 1996; Keller 1997; Pyrak-Nolte et al. 1997; Brown et al. 1998; Keller 1998; Djik et al. 1999; Bertels et al. 2001) and that roughness of the fracture walls is often fractal (Poon et al. 1992; Roux et al. 1993; Schmittbuhl et al. 1993; Brown 1995; Schmittbuhl et al. 1995; Boffa et al. 1998, 1999; Lanaro 2000; Plouraboué et al. 2000).

As variations in aperture size result in hydrodynamic dispersion and partial-flow channeling, the effects on solute transport are significant (cf. article 1). The accurate calculation of fluid velocities, therefore, must take into account the spatial distribution and size of the apertures. A rigorous approach should solve the 3-D Stokes' equation (see e.g., Mourzenko et al. 1995, 2001), but this is hardly conceivable whenever the study leaves the laboratory scale. The main reasons are:

– It is almost impossible to get a precise image of the geometric shape of natural fractures in situ.

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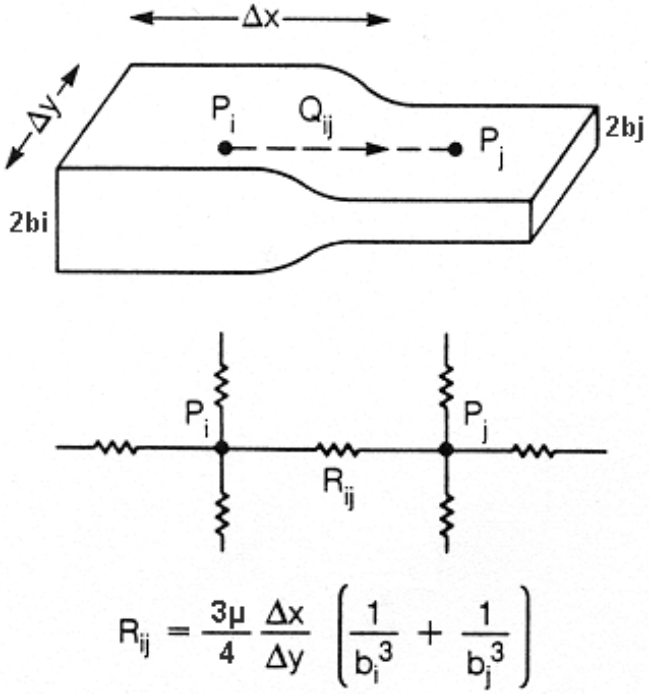

Fig. 3 Schematic diagram and electric analog for flow between two adjacent nodes of different apertures, b_i and b_j, in a single fracture [from Moreno et al. (1988), modified]. Reprinted from Water Resources Research 24(12), Moreno L, Tsang YW, Tsang CF, Hale FV, Neretnieks I, Flow and tracer transport in a single fracture: a stochastic model and its relation to some field observations, pp 2033–2048, Copyright (1988), with permission from American Geophysical Union

– The numerical resolution of the Stokes' equation requires complicated calculations that are beyond the computer capabilities when dealing with a fairly complex fracture network.

An approximation is then necessary and many authors assume that the "cubic" law is valid locally. In other words, in each point of the plane of a rough fracture, the cross-sectional profile of velocities is parabolic (Witherspoon et al. 1980; Moreno et al. 1988; Thompson and Brown 1991; David 1993; Unger and Mase 1993; Amadei and Illangasekare 1994; Plouraboué 1996; Lage 1997; Plouraboué et al. 1998; Roux et al. 1998; Cvetkovic et al. 1999). This 2-D simplification is also referred to as the Reynolds' approximation or the lubrication theory. A classical 2-D pressure-diffusion equation is obtained by coupling the Reynolds approximation with the mass-conservation principle. It describes the local fluid pressure in the fracture and is written in its simplified form as (Zimmerman and Bodvarsson 1996):

$$\frac{\partial}{\partial x}\left[b^3(x,y)\frac{\partial P}{\partial x}\right]+\frac{\partial}{\partial y}\left[b^3(x,y)\frac{\partial P}{\partial y}\right]=0 \qquad (14)$$

For a fracture with varying apertures, the pressure field is solved using a structured grid (i.e., meshes of regular size along each direction). Referring to Fig. 3, i and j are denoted as two adjacent nodes of the discrete grid along the x direction, and $2b_i$ and $2b_j$ are denoted as the local apertures. Using a harmonic mean for the inter-node transmissivity in expression (9) results in a pressure gradient between nodes i and j, which is:

$$\frac{\Delta P}{\Delta x}=\frac{Q_{ij}}{2\Delta y}\left(\frac{1}{2b_i^3/3\mu}+\frac{1}{2b_j^3\Big/3\mu}\right) \qquad (15)$$

that is:

$$P_i-P_j=Q_{ij}\left[\frac{3\mu}{4}\frac{\Delta x}{\Delta y}\left(\frac{1}{b_i^3}+\frac{1}{b_j^3}\right)\right]=Q_{ij}R_{ij} \qquad (16)$$

where R_{ij} is the resistance to the flow between nodes i and j (Fig. 3).

A mass-balance equation (Kirchoff's Law) is defined at each node i by:

$$\sum_j Q_{ij}=\sum_j\frac{P_i-P_j}{R_{ij}}=0 \qquad (17)$$

Knowing the boundary conditions and substituting expression (16) in (17) gives a linear system where the unknowns are the pressures at each node. Note also that Amadei and Illangasekare (1992) propose a semianalytical solution for flow that obviously avoids discretization. The solution is based on both the Louis extension of the cubic law [expression (12)] and a pressure estimate by Fourier series.

In a rough-walled fracture, the validity of the Reynolds' approximation can be discussed. Given the characteristics of Poiseuille's flow, it might be suggested that flow near the fracture walls is negatively influenced by their roughness. In fact, the zones of the fracture near the walls slightly participate in the fluid motion: for a pure parabolic cross-sectional profile of velocities, 10% of the total fracture volume adjacent to each wall merely transmits 5% of the total flow rate. Applying the nuclear magnetic resonance imaging (NMRI) technique, Djik and Berkowitz (1999) and Djik et al. (1999) were able to measure three-dimensional saturated flow fields in rough-walled fractures. The shape of the velocity profiles between the fracture walls was shown to be generally parabolic, as assumed by the Reynolds approximation, but not necessarily symmetrical. Djik et al. (1999) assert that the effects of this asymmetry on volumetric flow rates and hydraulic conductivities are insignificant, in that the overall flow inside rough fractures still obeys the cubic law. However, several theoretical and/or numerical studies showed that the Reynolds' approximation may fail with rough fractures and lead to non-negligible errors (Brown et al. 1995; Mourzenko et al. 1995; Ge 1997; Adler and Thovert 1999; Zimmerman and Yeo 2000). This was also revealed by experimental studies. For instance, Hakami and Larsson (1996) performed hydraulic tests and aperture measurements on a natural fracture in a granite core sampled at the Äspö site (Sweden). They found a measured mean aperture 1.4

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times the hydraulic aperture inferred from the cubic law. Amadei and Illangasekare (1994) and Larsson (1997) also showed an overestimation of 5–35% of the flow rates calculated with a simplified method using the mean aperture of a rough-walled fracture under a constant pressure gradient. Djik and Berkowitz (1999) also showed experimentally that in rough fractures with sharp fracture-wall discontinuities, the local cubic law may overestimate the actual flow rates because the 3-D flow is poorly approximated by a 2-D flow-rate estimate.

Several attempts have been undertaken to define the conditions for which the Reynolds' approximation is valid. Brown (1987, 1989), Oron and Berkowitz (1998), and Zimmerman et al. (1991) suggest that the principal condition relates to the local gradients of the aperture, which should be small (<<1). Zimmerman and Bodvarsson (1996) also state that the Reynolds number should be less than one in order to neglect inertial effects. The latter condition is confirmed by experiments in laboratory models of rough fractures (Nicholl et al. 1999). Finally, for Brown et al. (1995), Ge (1997) and Zimmerman and Bodvarsson (1996), the mean and the standard deviation of the apertures should be much smaller than the correlation length of the apertures in the fracture plane. However, it seems that even for an aperture/correlation length ratio below 0.1, the errors in the total flow rate due to the Reynolds approximation may be over 20% (Nicholl et al. 1999). According to Zimmerman and Yeo (2000), the Reynolds approximation (i.e. local cubic law) may suffice in estimating fracture permeability to within a factor of about two. More accurate estimates may require solving the 3-D Stokes' equations.

Unfortunately, when the Reynolds approximation is assumed, authors do not necessarily agree on the aperture to be used in the cubic law (Neuzil and Tracy 1981; Gelhar 1987; Mourzenko et al. 1995; Ge 1997; Lage 1997; Oron and Berkowitz 1998). The stochastic theory developed by Gelhar (1987) gives an effective transmissivity proportional to the geometric mean of the apertures, whereas the mean advection velocity of the solute is proportional to the arithmetic mean of the apertures. For Neuzil and Tracy (1981), a single aperture value is not sufficient to deal with flow in a rough fracture: other parameters such as the probability-density function of the apertures are necessary. Lage (1997) proposes a mathematical formalism of the cubic law based on the local aperture values and the tortuosity in the fracture plane. For Oron and Berkowitz (1998), the local aperture is useless and a mean calculated over a given length along the fracture is more valuable. The contact areas between the walls should also be accounted for. When they represent more than 5% of the total fracture plane, flow rapidly diverges from the cubic law.

Analytical Solutions to Advection–Dispersion

The analytical solution to expression (1) for an instantaneous injection at the inlet of the fracture corresponds to the classical solution to the advection–dispersion equation in a semi-infinite medium:

$$c_f(x,t) = \frac{m_0 x}{2bWu\sqrt{4\pi D_L t^3}} \exp\left(-\frac{(x-ut)^2}{4D_L t}\right) \tag{18}$$

with m_0 $[M]$ the injected mass; b $[L]$ the half-aperture of the fracture; and W $[L]$ the fracture width.

In the case of a continuous injection of constant concentration, the solution is the classical one given by Ogata and Banks (1961):

$$c_f(x,t) = \frac{c_0}{2}\left[erfc\left(\frac{x-ut}{2\sqrt{D_L t}}\right) + exp\left(\frac{ux}{D_L}\right) erfc\left(\frac{(x+ut)}{2\sqrt{D_L t}}\right)\right] \tag{19a}$$

with the following initial and boundary conditions:

$$c_f(x,0) = 0 \tag{19b}$$

$$c_f(0,t) = c_0 \tag{19c}$$

$$c_f(\infty,t) = 0 \tag{19d}$$

Expression (19a) simplifies if the ratio ux/D_L (i.e., the Peclet number) is large enough. It gives:

$$c_f(x,t) = \frac{c_0}{2} erfc\left(\frac{x-ut}{2\sqrt{D_L t}}\right) \tag{20}$$

The error, as compared with the complete solution, is about 3% for ux/D_L>500 (Silliman and Simpson 1987; Berkowitz et al. 1988). Note that several analytical solutions have also been developed for the case of a scale-dependent dispersion coefficient (Yates 1990, 1992; Huang et al. 1996; Pang and Hunt 2001).

The Taylor–Aris Dispersion

The dispersion coefficient calculated by Aris (1956), pursuing the work initiated by Taylor (1953), quantifies the solute dispersion in a tube under the combined effects of the parabolic cross-sectional profile of the fluid velocity and the molecular diffusion. Berkowitz and Zhou (1996) reassess the theory of flow and transport between parallel plates and find a transient dispersion coefficient whose asymptotic value is consistent with the previous work of Wooding (1960):

$$D_L = D_m + \frac{2}{105}\frac{u^2 b^2}{D_m} \tag{21}$$

where D_m $[L^2 \cdot T^{-1}]$ is the molecular-diffusion coefficient of the solute in free water (Einstein 1956):

$$D_m = \frac{k_B T}{6\pi\mu r_P} \tag{22}$$

with k_B $[M \cdot L^2 \cdot T^{-2} \cdot K^{-1}]$ as the Boltzmann constant ($1.38\ 10^{-23}$); T $[K]$ as the absolute temperature; μ $[M \cdot L^{-1} \cdot T^{-1}]$ as the dynamic viscosity; and r_P $[L]$ as the radius of the solute molecules.

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Note that Kessler and Hunt (1994) provide also an analytical expression for the asymptotic value of the Taylor–Aris dispersion coefficient in partially clogged fractures. Expression (21) shows that the Taylor–Aris dispersion varies with u^2 and b^2. In a parallel-plate system, the fluid velocity also varies with b^2 [see expression (8)]. Therefore, the Taylor–Aris dispersion is very sensitive to the fracture aperture since it is proportional to b^6.

It must be reminded that expression (21) is the asymptotic value of the dispersion coefficient, which is valid only beyond a critical travel time τ_c. This time corresponds to the minimum duration needed for a particle to experience the whole cross-sectional parabolic profile of velocities in the fracture. This critical time, therefore, is proportional to a characteristic time of transverse diffusion:

$$\tau_c \propto \frac{b^2}{D_m} \tag{23}$$

In other words, the solute must travel over a minimum distance x_c before the Taylor–Aris dispersion regime is completely established:

$$x_c >> u\tau_c \tag{24}$$

Wels et al. (1997) studied the combined effects of the Taylor–Aris dispersion and sorption reactions on the fracture walls. They showed with numerical simulations that τ_c should be corrected with a retardation factor, the Taylor–Aris regime being obtained beyond τ'_c :

$$\tau'_c = R_a\tau_c \tag{25}$$

Following Berkowitz and Zhou (1996), the complete transient expression of the dispersion coefficient can be developed as:

$$D_L = D_m + \frac{u^2b^2}{D_m}\left[\frac{2}{105} - \sum_{n=1}^{\infty}\frac{18}{(n\pi)^6}\exp\left(-\frac{n^2\pi^2D_m}{b^2}t\right)\right] \tag{26}$$

Replacing the time t by τ_c leads rapidly to negligible terms in the sum of expression (26) and results in the Taylor–Aris dispersion coefficient [expression (21)].

Hydrodynamic Dispersion in a Fracture with Variable Aperture

The stochastic development by Gelhar (1993) of the transport equations provides an approximation of the equivalent homogeneous dispersion in a fracture with variable aperture. This dispersion is characterized by the longitudinal macrodispersivity, which is:

$$\alpha_g = \left[3 + G(\sigma_\beta)\right]\sigma_\beta^2\lambda_\beta \tag{27}$$

where:

$$G(\sigma_\beta) = 1 + 0.205\sigma_\beta^2 + 0.16\sigma_\beta^4 + 0.045\sigma_\beta^6 + 0.115\sigma_\beta^8 \tag{28}$$

for $0 < \sigma_\beta < \sqrt{5}$; where λ_β [L] and σ_β [-] are the correlation length and the standard deviation of the logarithm of the apertures [ln(2b)], respectively. This model is based on the following assumptions:

- A weak local dispersivity as compared with the correlation length of the apertures.
- A statistically homogeneous logarithm of the apertures with a spatial structure following an exponential variogram:

$$\gamma(h) = \sigma_\beta^2\left[1 - \exp\left(-\frac{h}{\lambda_\beta}\right)\right] \tag{29}$$

As for the Taylor–Aris dispersion, expression (27) is an asymptotic value. It assumes fully developed dispersion in the fracture, i.e., a transport distance of more than ten correlation lengths λ_β. Keller et al. (1995, 1999) tested this model by comparing its results to dispersivity values calculated from laboratory experiments in natural fractures (cores). The differences between theory and experiments are in the order of 33–100% and are supposed to be the consequence of experimental uncertainties and channeling effects not taken into account in the theoretical model. Detwiler et al. (2000) also observed some discrepancies between the theoretical model predictions and the dispersion estimated from laboratory experiments in rough-walled fracture made of two pieces of textured glass. They invoked deviations from the Reynolds' approximation for computing the flow in their experimental rough fracture.

Transition Between the Dispersion Regimes

As stated in the first article, the effects of molecular diffusion, Taylor–Aris dispersion, and aperture variation dispersion add up in a natural fracture. Detwiler et al. (2000) developed analytical expressions for predicting the dominant dispersion mechanism for a given statistical distribution of the fracture apertures and flowing conditions. The Peclet number is here defined as:

$$P_e = \frac{u\langle 2b\rangle}{D_m} \tag{30}$$

where u [$L{\cdot}T^{-1}$] is the mean-solute velocity and $\langle 2b\rangle$ [L] is the mean-fracture aperture. The transition from diffusion regime to aperture–variation dispersion is reached for:

$$P_e \geq \frac{\langle 2b\rangle}{\sigma_\beta^2\lambda_\beta\left[3 + G(\sigma_\beta)\right]} \tag{31}$$

with σ_β, λ_β and $G(\sigma_\beta)$ as defined for expression (28). The transition from aperture-variation dispersion to Taylor–Aris dispersion regime is reached for:

$$P_e \geq \frac{210\sigma_\beta^2\lambda_\beta\left[3 + G(\sigma_\beta)\right]}{\langle 2b\rangle} \tag{32}$$

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Modeling the Scale Effects of Dispersion

The asymptotic behavior predicted by theoretical models of dispersion is often questioned in view of many experimental results (cf. article 1). An increase in dispersivity with the travel distance is often visible beyond the critical distances predicted by the theory. This inconsistency is interpreted by most authors as a scale effect stemming from flow channeling in the fracture plane. Unfortunately, the modeling of this phenomenon is often undertaken following divergent concepts.

Molz et al. (1983) advocate a thorough characterization of the local scale heterogeneity, in other words a fine discrete approach to channeling. Although rigorous, this approach comes up against the same computation efforts as those evoked in the flow calculation (cf. section on Laminar Flow in a Fracture with Varying Aperture). Because the geometry of natural fractures in situ cannot be defined and the calculations are too complicated, the method is inconceivable at the scale of a natural-fracture network. A macroscopic approach to the scale effect of channeling appears more realistic. Thus, some authors consider dispersion as a function of the migration distance (or of the mean travel time). This requires one to rewrite the transport equation in the fracture as [expression (1)]:

$$\frac{\partial c_f}{\partial t} = \frac{\partial}{\partial x}\left(D_L \frac{\partial c_f}{\partial x}\right) - u\frac{\partial c_f}{\partial x} \tag{33}$$

Note that Berkowitz and Scher (1995) showed that the use of a scale- or time-dependent dispersion coefficient contradicts the fundamental assumptions used to develop the conventional transport equations. However, classical equations such as expression (33) remain widely used for practical cases. Pickens and Grisak (1981) propose several models of varying dispersion:

$$-\text{The linear model}: \quad \alpha_{\mathrm{L}} = \omega x \tag{34}$$

$$-\text{The power law model}: \quad \alpha_{\mathrm{L}} = \omega x^{\xi} \tag{35}$$

$$-\text{The asymptotic model}: \quad \alpha_L = \Psi\left(1 - \frac{\eta}{x+\eta}\right) \tag{36}$$

$$-\text{The exponential model}: \quad \alpha_L = \Phi[1 - \exp(-\kappa x)] \tag{37}$$

with ω [-]; ξ [-]; κ [L^{-1}] as constants; Ψ [L] as the asymptotic dispersivity; η [L] as the migration distance for which dispersivity is half the asymptotic value; and Φ [L] as the maximal value of dispersivity in the exponential model.

The power-law model was used by Neuman (1990, 1994) to fit 131 dispersivity values as functions of the migration distance. Most of the reference tracer tests were performed over distances between 1–10^3 m, and concern both porous and fractured media. They follow the same power law for the dispersivity versus migration distance and the best fit, with a correlation factor of 0.75, corresponds to the expression:

$$\alpha_L = 0.017x^{1.5} \tag{38}$$

This scale effect is interpreted by Neuman as the consequence of the fractal nature of the hydraulic-conductivity field. This concept of a relation between the scale effect of dispersion and the fractal organization of the medium is also defended by Wheatcraft and Tyler (1988). Similarly to Neuman's approach, Gelhar et al. (1992) propose another study of the scale effect from a critical review of dispersivity values measured in fractured and porous media. The general trend of an increase in dispersivity with the transport distance is also shown, but, contrary to Neuman, the fitting cannot be done with a unique universal law. Gelhar et al. favor a scale law as a function of the spatial structure of the hydraulic conductivity, but specific to each medium.

Modeling of Reactive Transport in a Single Fracture

Reversible Sorption Reactions

A sorption reaction is characterized by a partition coefficient that expresses the ratio between the adsorbed mass onto the solid and the mass in the fluid. Consider the following reaction: $\phi_{aq} \leftrightarrow \phi_s$ where ϕ_{aq} is the element in solution in the fluid and ϕ_s is the element in the solid. For linear equilibrium, the partition coefficient is written (Freeze and Cherry 1979):

$$K_d = \left.\frac{[\varphi]_s}{[\varphi]_{aq}}\right|_{eq} \tag{39}$$

with $[\phi_s]$ the concentration of the element in the solid phase, expressed as a mass per unit surface [$M{\cdot}L^{-2}$] for a sorption on the fracture walls, or as a mass per unit mass of solid [$M{\cdot}M^{-1}$] for sorption onto the matrix; and $[\phi_{aq}]$ the concentration in the fluid phase, expressed as a mass per unit volume [$M{\cdot}L^{-3}$].

Therefore, the sorption coefficient K_d is expressed either as [L] (surface-sorption coefficient) or as [$L^3{\cdot}M^{-1}$] (volumetric-sorption coefficient). As pointed out by Neretnieks (1993), sorption reactions may stem from various mechanisms and complex processes can intervene in the rock–solute interactions (cf. article 1). Therefore, K_d is a very vague notion, but remains widely used in models because of its simplicity.

For instantaneous equilibrium, the derivative of expression (39) with respect to time yields:

$$\frac{\partial[\varphi]_s}{\partial t} = K_d \frac{\partial[\varphi]_{aq}}{\partial t} = K_d \frac{\partial c}{\partial t} \tag{40}$$

In the case of a single fracture with an impervious matrix, sorption reactions are limited to the fracture walls and the sorption effect in the transport equation is expressed by the addition of a source term to expression (1) [or to expression (33) if dispersion is not constant]:

$$\frac{\partial c_f}{\partial t} + a_w K_d \frac{\partial c_f}{\partial t} = D_L \frac{\partial^2 c_f}{\partial x^2} - u\frac{\partial c_f}{\partial x} \tag{41}$$

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where a_w [L^{-1}] is the ratio between the wall surface in contact with the solute and the volume of fluid in the fracture plane. This term is also called the "flow wetted surface" (Moreno and Neretnieks 1993a) or the "specific surface area" (Wels et al. 1996). For a parallel-plate fracture, it is expressed as:

$$a_w = \frac{1}{b} \tag{42}$$

For a natural fracture likely to present contact areas between the walls or flow channeling, it gives:

$$a_w \leq \frac{1}{b} \tag{43}$$

At the field scale, the flow-wetted surface can be estimated from the mean number of flowing fractures intersecting a unit length of a borehole (Gylling et al. 1998, see article 1, section on Factors of influence to Matrix Diffusion).

In order to account for the delay by sorption on the migration of a reactive solute in comparison with the migration of a non-reactive one, a retardation factor is defined as follows:

$$R_f = 1 + a_w K_d \tag{44}$$

This allows one to rewrite expression (41) as follows:

$$\frac{\partial c_f}{\partial t} = \frac{D_L}{R_f}\frac{\partial^2 c_f}{\partial x^2} - \frac{u}{R_f}\frac{\partial c_f}{\partial x} \tag{45}$$

As shown in expression (45), the retardation factor applies in the same manner to both advective and dispersive fluxes. Expressions (42) and (44) show that the retardation "intensity" is inversely related to the fracture aperture. This relation was verified experimentally by Wels et al. (1996). But these authors also suggest the existence of a relationship: K_d=$f(a_w)$, which expresses a positive correlation between the sorption strength and the fracture aperture. This could explain some experimental observations such as the abnormally strong influence of the fracture aperture on the solute retardation. In the case where both the aperture and the partition coefficient vary in space, Gelhar (1987) demonstrates that an effective retardation factor can be defined using the arithmetic means of the aperture and of the partition coefficient.

Expressions (39) to (45) are valid for simple-reactive transport with instantaneous linear equilibrium. Sometimes, sorption reactions are better represented by means of a non-linear isotherm such as the Freundlich [expression (46)] or Langmuir ones [expression (47)]:

$$[\varphi]_s = K_d [\varphi]_{aq}^{\beta_F} \tag{46}$$

$$[\varphi]_s = \frac{[\varphi]_s^0 K_d [\varphi]_{aq}}{1 + K_d [\varphi]_{aq}} \tag{47}$$

with β_F [-] as the Freundlich exponent, generally in the range 0.7–1.2 (Banton and Bangoy 1997); and $[\varphi]_s^0$ as the maximal concentration adsorbed onto the solid phase.

In these conditions, transport may become complex because the nature of the reaction and its intensity depend on the local solute concentration in the fracture. The problem may be quite linear over a given range of concentrations and become non-linear for another range.

Generally, equilibrium between the solute in the fluid and the adsorbed mass is very rapid as compared with the characteristic time of transport. Therefore, the assumption of instantaneous reactions is reasonable. However, several experiments have shown that kinetics are sometimes slow and/or different between the adsorption and desorption processes (cf. article 1). These observations are often modeled with first-order kinetics:

$$\frac{\partial [\varphi]_s}{\partial t} = k_{ads}[\varphi]_{aq} - k_{dsp}[\varphi]_s \tag{48}$$

with k_{ads} [$L \cdot T^{-1}$] or [$L^3 \cdot M^{-1} \cdot T^{-1}$] ; k_{dsp} [T^{-1}] as adsorption and desorption rates, respectively.

The transport equation, including the effects of first-order kinetics in a parallel-plate fracture, is detailed by Berkowitz and Zhou (1996). These authors emphasize interesting criteria to distinguish between reactive/non-reactive solutes or reversible/non-reversible reactions or local equilibrium/first-order kinetics.

Decay Reactions

Several types of reactions are able to induce a decrease over time in the solute mass. The first example is a radioactive element subjected to natural decay. Some solutes can also be adsorbed irreversibly onto the fracture walls or undergo biodegradation reactions. Generally, decay reactions obey first-order kinetics, which is written as:

$$\frac{\partial c}{\partial t} = -\lambda c \tag{49}$$

where λ [T^{-1}] is the decay constant. The half-life period is commonly used as a characteristic of the reaction and is written:

$$t^{1/2} = \frac{\ln 2}{\lambda} \tag{50}$$

The transport equation with both instantaneous reversible sorption and mass decay is written as:

$$\frac{\partial c_f}{\partial t} + \lambda c_f = \frac{D_L}{R_f}\frac{\partial^2 c_f}{\partial x^2} - \frac{u}{R_f}\frac{\partial c_f}{\partial x} \tag{51}$$

The degradation of some chemical species or classical radioactive decay can be accompanied by the appearance of new species. This process is referred to as a decay chain reaction. Note that it may also affect organic solutes. A transport equation must then be written for each element in solution (Huyakorn et al. 1983b). For an element indexed as j, this gives:

$$\frac{\partial c_f^j}{\partial t} + \lambda_j c_f^j = \frac{D_L}{R_f^j}\frac{\partial^2 c_f^j}{\partial x^2} - \frac{u}{R_f^j}\frac{\partial c_f^j}{\partial x} + \sum_{i=1}^{M} \zeta_{ij}\frac{R_f^i}{R_f^j}\lambda_i c_f^i \tag{52}$$

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with c_f^i, c_f^j [$M \cdot L^{-3}$] as the concentration of elements i and j in solution; R_f^i, R_f^j [-] as the retardation coefficient of elements i and j; ζ_{ij} [-] as the fraction of parent element i transformed into element j; M [-] as the total number of parent elements i transformed into element j; and λ_i, λ_j [T^{-1}] as the decay constant of elements i and j.

Matrix Diffusion

Even for a medium of low matrix porosity (less than 5%), solute exchanges between fractures and the neighboring matrix are often non-negligible (cf. article 1). Matrix diffusion is generally regarded as a 1-D process. This assumption is justified if one considers that the solute migration is much faster in fractures than in the matrix. Diffusive exchanges along the direction parallel to the fracture plane are then negligible as compared with those perpendicular to the fracture plane (which is also the direction of the maximal concentration gradient). Kennedy and Lennox (1995) showed numerically that this assumption holds in most cases, but may be erroneous for instance in fractured clay with fracture apertures of less than 20 μm and flow velocities lower than 1 m/day.

The evolution of the solute concentration within the matrix obeys the second Fick's law (Crank 1980), which writes in 1-D:

$$\frac{\partial c}{\partial t} = D_a \frac{\partial^2 c}{\partial z^2} \tag{53}$$

where D_a [$L^2 \cdot T^{-1}$], the apparent-diffusion coefficient, is considered as a constant. The diffusion coefficient depends on both the solute nature and the problem scale. Denoting D_m as the molecular-diffusion coefficient of the solute in free water [expression (22)], Ohlsson and Neretnieks (1995) distinguish between two scales:

1. At the scale of a few connected pores, the pore-diffusion coefficient D_p includes the resistance to diffusion stemming from the pore geometry ($D_p < D_m$). See Eq. (54), where δ_D [−] is the pore constrictivity; and τ^2 [−] is the pore tortuosity:

$$D_p = \frac{\delta_D}{\tau^2} D_m \tag{54}$$

2. At the scale of the rock matrix, the effective-diffusion coefficient D_e includes the effects of porosity through a formation factor F_f (Neretnieks 1993). The diffusion equation can be written as Eq. (55), where D_e is defined as in Eq. (56), with θ_m [−] the matrix porosity separated into transport porosity θ_t and storage porosity θ_s (Eq. 57); and F_f [−] the formation factor (Eq. 58):

$$\theta_m \frac{\partial c_m}{\partial t} = \frac{\partial}{\partial z}\left(D_e \frac{\partial c_m}{\partial z}\right) \tag{55}$$

$$D_e = \theta_t D_p = F_f D_m \tag{56}$$

$$\theta_m = \theta_t + \theta_s \tag{57}$$

$$F_f = \frac{\theta_t \delta_D}{\tau^2} \tag{58}$$

The formation factor can be evaluated experimentally using the technique proposed by Skagius and Neretnieks (1986a; cf. article 1, section on Channeling). Sato (1999) also proposes an empirical relation between the formation factor and the porosity obtained from through-diffusion experiments and mercury-porosimeter measurements in samples of crystalline rocks:

$$F_f = \theta_m^{1.57 \pm 0.02} \tag{59}$$

A similar power-law relation was found by Boving and Grathwohl (2001) from through-diffusion experiments in sedimentary rocks (limestone and sandstone), but with an exponent of 2.2 instead of 1.57.

With a solute that undergoes sorption and/or decay reactions, the diffusion equation in the matrix is rewritten as (Grisak and Pickens 1980; Skagius and Neretnieks 1986b):

$$\left[\frac{\partial c_m}{\partial t} + \lambda c_m\right](\theta_m + K_d \rho_m) = \frac{\partial}{\partial z}\left(D_e \frac{\partial c_m}{\partial z}\right) \tag{60}$$

To account for the potential mobility by diffusion of the solute in the sorbed phase, the concept of "surface diffusion" may be introduced (Ohlsson and Neretnieks 1995; Xu and Wörman 1999). It handles different diffusion coefficients between the free and the adsorbed concentrations:

$$\theta_m\left[\frac{\partial c_m}{\partial t} + \lambda c_m\right] + \rho_m\left(\frac{\partial c_s}{\partial t} + \lambda c_s\right) = \frac{\partial}{\partial z}\left(\rho_m D_s \frac{\partial c_s}{\partial z} + D_e \frac{\partial c_m}{\partial z}\right) \tag{61}$$

where $c_s = K_d c_m$, is the concentration of the sorbed solute in the solid phase [$M \cdot M^{-1}$], and D_s [$L^2 \cdot T^{-1}$] is the diffusion coefficient in the sorbed phase. Note that D_s is, in general, concentration dependent:

$$D_s = f(c_s) \tag{62}$$

Neglecting surface diffusion and considering the case of homogeneous diffusion in the matrix, Eq. (60) is simplified as:

$$\frac{\partial c_m}{\partial t} + \lambda c_m = D_a \frac{\partial^2 c_m}{\partial z^2} \tag{63}$$

where:

$$D_a = \frac{D_e}{\alpha} \tag{64}$$

and α [-] is the capacity factor including the sorption properties of the matrix. For a reversible-sorption reaction and an instantaneous equilibrium with linear isotherm, this factor is expressed as (Ohlsson and Neretnieks 1995):

$$\alpha = \theta_m + K_d \rho_m \tag{65}$$

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where K_d [$L^3 \cdot M^{-1}$] is the volume sorption coefficient; and ρ_m [$M \cdot L^{-3}$] is the bulk density of the rock.

For the same reaction, but with a Freundlich isotherm, the capacity factor is expressed as (Ohlsson and Neretnieks 1995):

$$\alpha = \theta_m + K_d \rho_m \beta_F c_m^{\beta_F - 1} \tag{66}$$

with β_F [-] as the Freundlich exponent.

In reality, the assumption of a constant-diffusion coefficient in the matrix is questionable. Altered zones and/or microfractures are often observed near the fracture walls and they can increase the matrix diffusion as compared to the non-altered massive rock located a few centimeters deeper (Skagius and Neretnieks 1986b). In the general case, where there are variations in the matrix block geometry and in the diffusion coefficient with the depth from the fracture plane, the diffusion equation can be written (Neretnieks and Rasmuson 1984; Rasmuson and Neretnieks 1986):

$$\frac{\partial c_m}{\partial t} + \lambda c_m = \frac{1}{\alpha A} \frac{\partial}{\partial z} \left(D_e A \frac{\partial c_m}{\partial z} \right) \tag{67}$$

where $A(z)$ is the cross-sectional area of the matrix block normal to the transport direction in the fracture. There are no analytical solutions to expression (67), which must be solved numerically. Carrera et al. (1998) have used a convolution approach with a "memory function" of the system and have shown that the matrix-block geometry is of secondary importance in the fracture/matrix exchanges. For easier cases, Carslaw and Jaeger (1959) and Crank (1980) propose analytical solutions. Thus, with a constant-exchange area, a constant-diffusion coefficient [expression (63)] and a non-reactive solute or linear reversible instantaneous sorption [Eq. (65)], the matrix diffusion is solved by:

$$c_m(z,t) = c_0 \operatorname{erfc}\left(\frac{z-b}{\sqrt{4 D_a t}} \right) \exp(-\lambda t) \tag{68a}$$

with $b \leq z < \infty$; for a continuous injection into the fracture (i.e. a constant concentration in the fracture in $z=b$ or a decreasing one, following a first-order decay), and the following initial and boundary conditions:

$$c_m(z,0) = 0 \tag{68b}$$

$$c_m(b,t) = c_0 \exp(-\lambda t) \tag{68c}$$

$$c_m(\infty,t) = 0 \tag{68d}$$

The matrix diffusion is also solved by the following expression:

$$c_m(z,t) = \frac{m_0}{\sqrt{\pi D_a t}} \exp\left(-\frac{(z-b)^2}{4 D_a t} \right) \exp(-\lambda t i g h t) \tag{69a}$$

with $b \leq z \leq \infty$; for an instantaneous injection into the fracture, which may lead to the instantaneous inlet of a mass m_0 in the matrix at $t=0$ in $z=b$, and the following initial and boundary conditions:

$$c_m(z,0) = 0 \tag{69b}$$

$$c_m(\infty,t) = 0 \tag{69c}$$

Given the boundary conditions (68d) and (69c), these analytical solutions are strictly valid for a semi-infinite medium and they imply non-limited diffusion into the matrix. The latter assumption is commonly used by several authors (Grisak and Pickens 1981; Moreno and Neretnieks 1993b; Küpper et al. 1995a, 1995b; Selroos and Cvetkovic 1996; Hölttä et al. 1997; Wallach and Parlange 1998). However, matrix blocks are of finite size and the assumption of an infinite matrix should be discussed. Its validity depends on the maximal depth of penetration of the solute into the matrix. In fact, the solute motion from a fracture into the matrix should not be influenced by the fluxes from other fractures. For instance, in a system of parallel fractures, the infinite-matrix assumption is relevant if the solute does not move beyond the central line of the inter-fracture blocks. Therefore, a rigorous use of the infinite-matrix assumption is subjected to constraints on:

- The shape and size of the matrix blocks.
- The duration of the injection.
- The value of the apparent diffusion coefficient.

Considering an apparent diffusion coefficient $D_a = 10^{-10}$ m^2 s^{-1} and a fracture spacing of 10 m, Grisak and Pickens (1981) have shown that matrix diffusion could be reasonably considered as non-limited in rocks of very low porosity (less than 0.5%), even in case of long-term injections (several hundred years). In rocks with higher porosity, such as chalk, and a small fracture spacing (in the order of 0.1 m), Maloszewski and Zuber (1985) have shown that the infinite-matrix assumption is only valid for short-term injections (a few days to one month). The assumption of concentration equilibrium between the fractures and the rock matrix was used by Cook et al. (1996), who studied the chlorofluorocarbon and ^{3}H/^{3}He profiles in fractured-rock aquifers of the Oak Ridge Reservation (ORR), Tennessee, USA. This assumption was revealed to be valid in the upper part of the flow system, made of highly weathered shales with a fracture spacing of less than 5 cm, but was not realistic in the lower flow system, made of unweathered shales and limestones with a fracture spacing between 2–5 m.

Dershowitz and Miller (1995) provide an analytical solution to the matrix diffusion of a non-reactive solute in finite-size blocks:

$$c_m(z,t) = \frac{2 c_0}{\pi} \sum_{n=1}^{\infty} \left[\frac{1}{n} \sin\left(\frac{b}{B} n\pi \right) \cos\left(\frac{z}{B} n\pi \right) \cdot \cdot \exp\left(-n^2 \pi^2 \frac{D_a t}{B^2} \right) \right] \tag{70a}$$

for $b \leq z < B$; with b [L] as the half-aperture of the fracture; and B [L] as the maximal depth of penetration by diffusion.

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The initial and boundary conditions associated with expression (70a) are:

$$c_m(z,0) = 0 \tag{70b}$$

$$c_m(b,t) = c_0 \tag{70c}$$

$$\text{at } z = B, \text{for } t > 0, \frac{\partial c_m}{\partial z} = 0 \tag{70d}$$

Coupling of Transport in Fractures and Matrix Diffusion

In the fracture, the diffusive exchanges with the matrix are modeled by an additional source term. The transport equation in the fracture is written (Tang et al. 1981; Moreno et al. 1985):

$$\frac{\partial c_f}{\partial t} + \lambda c_f = \frac{D_L}{R_f}\frac{\partial^2 c_f}{\partial x^2} - \frac{u}{R_f}\frac{\partial c_f}{\partial x} + \frac{a_w D_e}{R_f}\frac{\partial c_m}{\partial z}\bigg|_{z=b} \tag{71}$$

Analytical solutions to the coupling of (71) and (63), (64), and (65) are given by Tang et al. (1981). For a continuous injection of constant concentration in a parallel-plate fracture, one gets in the fracture:

$$c_f(x,t) = \frac{c_0}{\sqrt{\pi}}\exp(\nu x)\int_l^\infty \exp\left(-\xi^2 - \frac{\nu^2 x^2}{4\xi^2}\right)\cdot \cdot \exp\left(-\eta x^2\right)\left\{\exp\left(-Y\sqrt{\lambda}\right)\operatorname{erfc}\left(\frac{Y}{2T} - T\sqrt{\lambda}\right) + \exp\left(Y\sqrt{\lambda}\right)\operatorname{erfc}\left(\frac{Y}{2T} + T\sqrt{\lambda}\right)\right\}d\xi \tag{72a}$$

in the matrix:

$$c_m(x,t) = \frac{c_0}{\sqrt{\pi}}\exp(\nu x)\int_l^\infty \exp\left(-\xi^2 - \frac{\nu^2 x^2}{4\xi^2}\right)\cdot \cdot \exp\left(-\eta x^2\right)\left\{\exp\left(-Y'\sqrt{\lambda}\right)\operatorname{erfc}\left(\frac{Y'}{2T} - T\sqrt{\lambda}\right) + \exp\left(Y'\sqrt{\lambda}\right)\operatorname{erfc}\left(\frac{Y'}{2T} + T\sqrt{\lambda}\right)\right\}d\xi \tag{72b}$$

where:

$$\nu = \frac{u}{2D_L} \tag{72c}$$

$$l = \frac{x}{2}\sqrt{\frac{R_f}{D_L t}} \tag{72d}$$

$$Y = \frac{\nu^2\beta^2 x^2}{4\Gamma\xi^2} \tag{72e}$$

$$Y' = \frac{\nu^2\beta^2 x^2}{4\Gamma\xi^2} + (z-b)\sqrt{\frac{\alpha}{D_e}} \tag{72f}$$

$$\beta = \frac{2}{u}\sqrt{R_f D_L} \tag{72g}$$

$$\Gamma = \frac{bR_f}{\sqrt{\alpha D_e}} \tag{72h}$$

$$T = \sqrt{t - \frac{\nu^2\beta^2 x^2}{4\xi^2}} = \sqrt{t - \frac{R_f x^2}{4D_L\xi^2}} \tag{72i}$$

$$\eta = \frac{\lambda R_f}{4D_L\xi^2} \tag{72j}$$

This solution was extended by Moreno and Rasmuson (1986) to the case of a continuous injection of constant-mass flux. For an instantaneous injection and reversible instantaneous sorption in the fracture, the following solution is given by Maloszewski and Zuber (1990):

$$c_f(x,t) = \frac{m_0 a}{2\pi Q}\sqrt{P_e t'_0}\int_0^t \exp\left(-\frac{P_e\left(t'_0 - \psi\right)^2}{4\psi t'_0} - \frac{a^2\psi^2}{t-\psi}\right)\frac{d\psi}{\sqrt{\psi(t-\psi)^3}} \tag{73a}$$

where:

$$a = \frac{\alpha}{2bR_f}\sqrt{D_a} \tag{73b}$$

m_0 [M] is the injected mass; P_e [-] is the Peclet number:

$$P_e = \frac{ux}{D_L} \tag{73c}$$

t'_0 [T] is the mean-residence time in the fracture:

$$t'_0 = R_f\frac{x}{u} \tag{73d}$$

Note that Maloszewski and Zuber (1990) also give a general solution that is able to deal with first-order kinetics for sorption reactions in the matrix.

Other solutions are available in the literature. They refer to various assumptions such as negligible dispersion in the fracture (Neretnieks 1980; Grisak and Pickens 1981), or matrix-fracture exchange controlled by diffusion through a stagnant-fluid layer at the interface (Wallach and Parlange 1998). Some solutions have also been developed for specific geometry or boundary conditions. For instance: injection into a well and radial flow (Feenstra et al. 1984; Chen 1985, 1986; Novakowski 1992), injection imposed in terms of a flux of finite mass (Fujikawa and Fukui 1990), sources of solute in the porous matrix (Homp and Logan 1997), non-equilibrium sorption in the matrix (Lee and Teng 1993), and radioactive-decay chain (Sudicky and Frind 1984; Cormenzana 2000). Some of these solutions are given in the Laplace space so a numerical inversion is needed to obtain a result in the real space.

A lot of solutions have been developed for systems of parallel equidistant fractures of constant aperture as that illustrated in Fig. 4. As stated above, diffusion is modeled as a 1-D process, but the solute motion in the matrix does not extends beyond the central axis of the matrix blocks. For a continuous injection at the inlet of the fractured system, Barker (1982) and Sudicky and Frind (1982)

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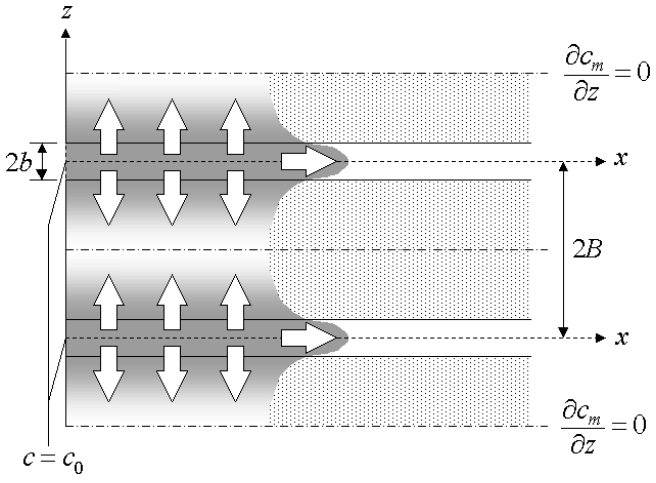

Fig. 4 Schematic representation of solute transport in a system of parallel fractures with a constant source input c_o and no flux conditions at the center of matrix blocks

propose their analytical solutions in the Laplace space. Sudicky and Frind (1982) also give a solution in the real space, but it includes a double integral of an oscillatory function whose numerical evaluation is problematical. The advice of Pinder et al. (1993) is to proceed with the numerical inversion of the Laplace-space solution by following a scheme described by Crump (1976):

$$c_f(x,t) \approx \frac{1}{T^*}\exp(p_0 t)\left[\frac{1}{2}\bar{c}_f(x,p_0) + \sum_{k=1}^{2N+1}\left[\mathrm{Real}\left[\bar{c}_f(x,p_k)\right]\cdot \cos\left(\frac{k\pi t}{T^*}\right) - \mathrm{Im}\left[\bar{c}_f(x,p_k)\right]\sin\left(\frac{k\pi t}{T^*}\right)\right]\right] \quad (74a)$$

where:

$$p_0 = -\frac{\ln(E)}{2T^*} \quad (74b)$$

$$p_k = p_0 + i\frac{k\pi}{T^*} \quad (74c)$$

and $\bar{c}_f$ is the solution of Sudicky and Frind in the Laplace space:

$$\bar{c}_f = \frac{c_0}{P-\lambda}\exp(\nu x)\cdot \cdot \exp\left(-\nu x\sqrt{1+\kappa^2\left(\frac{\sqrt{P}}{\Gamma}\tanh\left(\sigma\sqrt{P}\right)+P\right)}\right) \quad (75a)$$

where ν is defined as Eq. (72c) and Γ is defined as Eq. (72h).

$$P = p + \lambda \quad (75b)$$

$$\kappa^2 = \frac{4R_f D_L}{u^2} \quad (75c)$$

$$\sigma = \frac{B-b}{\sqrt{D_a}} \quad (75d)$$

with p the Laplace parameter; $2T^*$ the period of the Fourier series approximating the inverse function; E [$M{\cdot}L^{-3}$] the absolute error tolerance; $2N{+}1$ the number of Fourier harmonics in the decomposition of $\bar{c}f$; $i = \sqrt{-1}$; *Real*, *Im* the real and imaginary parts of a complex number, respectively.

It must be noted that the accuracy of the numerical inversion increases with N. The period $2T^*$ must be over t_{max}, i.e., the maximal time beyond which the solution is no longer desired. A too-large value of T^* slows down the convergence and Crump (1976) found that $T^*{=}0{,}8t_{max}$ gives almost optimal results.

Maloszewski and Zuber (1985) propose an analytical solution in real space for the case of an instantaneous injection in a set of parallel fractures. Unfortunately, the complete solution is once again of limited interest because of the presence of the oscillatory integral mentioned above. Note, however, that the solution simplifies greatly if dispersion is neglected. According to Maloszewski and Zuber (1985), this approximation is relevant for fractured systems with high matrix porosity because transport is fully controlled by advection in fractures and by diffusion in the matrix. However, Tang et al. (1981) have observed that canceling fracture dispersion may result in important errors in case of low fluid velocity. The solutions developed by Barker (1982) and Sudicky and Frind (1982) theoretically correspond to parallel fractures of infinite length. These solutions have been extended to fractures of finite size by Robinson et al. (1998) and to 2-D and 3-D regular networks by Rowe and Booker (1989), (1990), and Rowe et al. (1989). The solutions proposed by Rasmuson and Neretnieks (1981), Rasmuson (1984), and Moench (1995) have been developed also for 3-D regular networks, but with attached spherical matrix blocks. Note that the solution by Moench (1995) assumes that the porous blocks are covered with a skin corresponding to a material of negligible volume and storage capacity, and that provides a resistance to diffusion in the rock matrix.

The interests of analytical solutions are to evaluate the relative influence of transport mechanisms on the one hand, and to provide some references for numerical codes on the other hand. Given the assumptions prevailing to their development, analytical solutions have a practical potential limited to problems with simple geometry. This is particularly emphasized for solutions of single-fracture transport problems. Consequently, the interpretation with analytical solutions of a tracer test performed in a single fracture may be justified (Novakowski and Lapcevic 1994), but the validity of the approach followed for instance by Maloszewski and Zuber (1990, 1992, 1993) is questionable: they use a solution developed for a single fracture (Maloszewski and Zuber 1985) to interpret field tracer tests performed in dense fractured rocks (tracer tests by Garnier et al. 1985; Cacas et al. 1990a). Himmelsbach et al. (1994, 1998) and Maloszewski et al. (1999) used the same method to interpret field-scale tracer tests in highly permeable fault and fracture zones. Maloszewski and Zuber acknowledge that their model is

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not realistic with respect to the fracture networks, but the single-fracture approximation is valid because matrix diffusion is, in their case study, the main governing transport process even in short-term tracer tests. Compared with other approaches such as EPM or discrete fracture network (DFN) modeling, the main advantage of the single fracture approach is the small number of parameters needed to fit the experimental breakthrough curves.

Other Approaches to the Coupled Fracture–Matrix Transport

The characteristic diffusion time in the matrix is generally much greater than the mean-travel time in the fracture. But if diffusion occurs only in a thin coat on the fracture walls (e.g., altered layer or precipitated deposits), the problem is inverted and the characteristic diffusion time may become lower than the travel time in the fracture. In the latter case, Neretnieks and Rasmuson (1984), and Rasmuson and Neretnieks (1986) have shown that the concept of the retardation factor can be used for modeling the effects of diffusion on transport. This procedure considerably simplifies the transport model by keeping an equation similar to that of a single fracture with impervious walls [Eq. (51)] instead of the complete coupling between the fracture and the matrix. With this approach, the retardation factor is expressed as a function of ρ_c as the bulk density of the coat; δ_c as its thickness; and a volumetric-sorption coefficient, K_d (Neretnieks and Rasmuson 1984):

$$R_a = 1 + \frac{\delta_c}{b} K_d \rho_c \tag{76}$$

Reedy et al. (1996) follow the approach by Coats and Smith (1964) to describe transport in laboratory columns of strongly altered and fractured shale. This well-known model is based on the "dual media" concept with a mobile-fluid fraction and an immobile one in dead-end pores. Transport in the mobile phase is governed by advection–dispersion mechanisms whereas exchanges with the immobile phase obey first-order kinetics:

$$\theta \frac{\partial c_f}{\partial t} + \theta' \frac{\partial c_{im}}{\partial t} = \theta D_L \frac{\partial^2 c_f}{\partial x^2} - \theta u \frac{\partial c_f}{\partial x} \tag{77a}$$

$$\theta' \frac{\partial c_{im}}{\partial t} = \omega \left(c_f - c_{im} \right) \tag{77b}$$

with c_f and c_{im} $[M \cdot L^{-3}]$ as the concentrations in the mobile (i.e., the fracture) and immobile (i.e., the matrix) phases, respectively; D_L $[L^2 \cdot T^{-1}]$ as the dispersion coefficient in the fracture; θ and θ' [-] as the volumetric fractions of the mobile and immobile phases, respectively; and ω $[T^{-1}]$ as the mass-transfer coefficient.

In order to reduce the differences between experimental results and simulations, Reedy et al. (1996) use a mass-transfer coefficient that decreases over time according to an exponential law:

$$\omega = \omega_0 \exp(-Rt) \tag{78}$$

However, they emphasize that Eq. (78) is not very easy to justify from a physical point of view. In fact, the Coats–Smith model seems to be valid only for short diffusion travels (Bibby 1981) and is not suited to numerous transport problems in fractured rocks where the migration distance into the matrix may reach about 1 m. Griffioen (1998) used analytical expressions to characterize the Fickian-diffusive flux for mass-transfer cycles in and out of stagnant layers. He showed that the first-order mass transfer concept cannot correctly describe diffusion if the cycle period is less than the characteristic time needed for filling completely the stagnant layer.

Heterogeneous Matrix Diffusion

As stated in the first report, the diffusive properties of the rock matrix could vary by one order of magnitude over very small distances (a few tens of centimeters). Most transport models do not address this problem and assume homogeneous diffusion. However, several recent studies, both numerical and analytical, showed that the spatial variations in the diffusive properties of the rock matrix could significantly modify the responses of the models. Considering a theoretical transport problem in a single fracture with variable apertures and heterogeneous matrix diffusion, Xu et al. (2001) have developed, within a stochastic framework, the analytical expressions of the mean and variance of the residence-time distribution. These expressions show that heterogeneity of fracture apertures and matrix diffusion do not affect the mean residence time, but increase the residence time variance. The "multiple-rate" model developed by Haggerty and Gorelik (1995, 1998) refers to the idea that, within a small volume of rock, multiple time scales of diffusion exist and operate simultaneously. A series of first-order equations is used to represent the solute exchanges between a mobile zone and any number of immobile zones of varying properties. This concept can thus apply to describe solute transport coupled with exchanges along a preferential flow path in a single fracture. This coupling may occur between the mobile fluid and the rock matrix or between the mobile fluid and stagnant water zones in the fracture plane (immobile zones). The coupled-transport equations are:

$$\frac{\partial c_f}{\partial t} = \frac{D_L}{R_f} \frac{\partial^2 c_f}{\partial x^2} - \frac{u}{R_f} \frac{\partial c_f}{\partial x} - \sum_{j=1}^{N} \beta_j \frac{\partial (c_{im})_j}{\partial t} \tag{79}$$

$$\frac{\partial (c_{im})_j}{\partial t} = \alpha_j \left[c_f - (c_{im})_j \right], \quad j = 1, 2, \ldots, N \tag{80}$$

with $(c_{im})_j$ $[M \cdot L^{-3}]$ as the aqueous concentration within the j^{th} immobile zone; β_j [-] as the ratio of total-solute mass in the immobile zone j, to the mass in the mobile zone at equilibrium; and α_j $[T^{-1}]$ as the apparent first-order mass transfer coefficient associated with the j^{th} immobile zone.

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According to Haggerty and Gorelik (1995), the parameters α_j and β_j should be considered a single distribution rather than two sets of *N*-independent parameters. This distribution might be statistically based, such as a uniform distribution, a lognormal distribution, or some other probability-density function characterized by a mean and a variance. Alternatively, the distribution may be physically based and directly related to diffusion. The authors showed that when using specific distributions of α_j, the multiple-rate model is (in reduced form) precisely equivalent to standard-diffusion models into/from spheres, cylinders, or layers. Note that this model has been used successfully for concrete case applications at the field scale by Haggerty (1999) and Haggerty et al. (2001).

Conclusion

This review has included the principal basic equations that describe solute transport at the scale of a single fracture and the neighboring porous matrix. The aim was to build a framework for modeling transport in fractured reservoirs following a discrete-fracture approach.

Among the physical mechanisms reviewed in the first article, channeling in the fracture plane is probably the most difficult to describe in terms of mathematical expressions. At the fracture scale, the problem is solvable: the fracture plane is discretized (either with a structured or a non-structured grid) to account for varying apertures and hence for varying fluid velocities from one location to the other (Moreno et al. 1988; Tsang et al. 1991; Amadei and Illangasekare 1994). At the network scale, Nordqvist et al. (1992) have proposed a 3-D model of flow and transport in fractures with varying apertures. They have introduced the single-fracture representation of Moreno et al. (1988) into the 3-D network model of Andersson and Dverstorp (1987). However, the matrix is assumed to be impervious, which prevents the simulation of potential matrix diffusion. Anyway, the use of this model for a problem at the scale of a reservoir is hardly conceivable because the number of fractures to be simulated is too high and cannot reasonably be handled given that each fracture is discretized. Moreover, it is hard enough to get information on the geometry of natural networks, but it is clearly impossible to characterize the statistical distribution of the fracture-plane apertures at the field scale.

Still in the scope of discrete modeling, other authors emphasize the formalism of transport equations at the scale of the preferential flow channels in the fracture plane. Therefore, the 3-D network is based on flowing bonds instead of fractures (Tsang and Tsang 1987; Cacas et al. 1990a, 1990b; Moreno and Neretnieks 1993b; Moreno et al. 1997; Gylling et al. 1998, 1999; Dershowitz and Fidelibus 1999). As for models with varying fracture apertures, the advantage claimed for this approach is the direct introduction of the channeling concept into the geometrical design of the model. Moreover, interactions are more easily modeled in the triple system: channels–matrix, channels–stagnant zones, stagnant zones–matrix (cf. article 1). The main difficulty remains to build the channel network associated with a given fracture network. Cacas et al. (1990a, 1990b) propose a simple but arbitrary method whereas Gylling et al. (1998) state that the geometric characteristics of channeling may be identified by the analysis of sampled cores and the performance of hydraulic tests over small distances on fractures insulated by packers in the wells.

In the more classical approach based on 2-D and 3-D fracture networks, the channeling effects must be integrated into the transport equations for each single fracture. One of the main consequences of channeling is the scale effect on dispersion, which can be handled by scale laws on dispersivity such as those proposed by Pickens and Grisak (1981; cf. section on Modeling of the Scale Effects of Dispersion). Note that this kind of approach is consistent with theoretical models such as the Taylor–Aris dispersion [expression (26)] or the macrodispersivity by Gelhar (1993) [expression (27)]. Some studies have been undertaken to circumvent the difficulty of handling anomalous dispersion with the classical advection–dispersion equation. These studies are often based on a stochastic approach to transport in the Lagrangian framework (Berkowitz and Scher 1998; Cvetkovic et al. 1999; Berkowitz et al. 2001; Kosakowski et al. 2001; Painter and Cvetkovic 2001). The aim is to calculate probability density functions for the presence of solute at a given location while accounting for the fluid-velocity heterogeneity and/or mechanisms such as matrix diffusion and sorption. There is no explicit reference to a dispersion coefficient; the spreading of solute is the result of the heterogeneity of flow and associated mechanisms. These approaches rely on non-obvious mathematical concepts and yield complex solutions to transport that are beyond the scope of this paper. They appear, however, as promising tools for further research in fractured media.

The other transport mechanisms (advection, sorption, matrix diffusion, decay reactions) are easier to describe. However, the resulting mathematical expressions do not lead to easy solutions, and the analytical ones are limited to "simple" cases. Modeling the solute migration in a realistic fractured media, while taking into account frequent mechanisms such as matrix diffusion, requires numerical methods. To limit the size of this review, this approach was deliberately overlooked.

The analytical solutions reported in this paper should be used to evaluate the relative influence of the various mechanisms that contribute to solute transport. They can also be seen as basic benchmarks for numerical methods. Their application to a practical case study at the field scale should be limited to the mere interpretation of a tracer test over a limited distance. It is obvious that the interest of analytical solutions remains very limited when dealing with transport problems developed over an entire fractured reservoir.

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Notation

c_f $[M{\cdot}L^{-3}]$ Volume concentration of solute in the fracture
t $[T]$ Time variable
x $[L]$ Space coordinate along the flow direction in the fracture plane
u $[L{\cdot}T^{-1}]$ Mean fluid velocity in the fracture
u_i $[L{\cdot}T^{-1}]$ Scalar component of the fluid velocity vector along the i direction ($i = x, y, z$)
D_L $[L^2{\cdot}T^{-1}]$ Hydrodynamic dispersion coefficient in the fracture
α_L $[L]$ Dispersivity in the fracture
D_m $[L^2{\cdot}T^{-1}]$ Molecular-diffusion coefficient of the solute in free water
Re [−] Reynolds number
ε $[L]$ Fracture roughness (mean height of the fracture asperity)
Rr [−] Relative roughness
b $[L]$ Half aperture of the fracture
W $[L]$ Width of the fracture in the direction perpendicular to the pressure gradient
υ $[L^2{\cdot}T^{-1}]$ Kinematic viscosity
μ $[M{\cdot}L^{-1}{\cdot}T^{-1}]$ Dynamic viscosity
D_h $[L]$ Hydraulic diameter of the fracture
S $[L^2]$ Flow section of the fracture
P_{ext} $[L]$ External perimeter of the flow section
ρ $[M{\cdot}L^{-3}]$ Mass density of the fluid
g_i $[L^2{\cdot}T^{-1}]$ Scalar component of the gravitational acceleration vector along the i direction (i=x, y, z)
$Q_{f\ unit}$ $[L^2{\cdot}T^{-1}]$ Flow rate per width unit in the fracture
Q_f $[L^3{\cdot}T^{-1}]$ Total flow rate in the fracture
P $[M{\cdot}L^{-1}{\cdot}T^2]$ Fluid pressure
H $[L]$ Hydraulic head
K_f $[L{\cdot}T^{-1}]$ Hydraulic conductivity of the fracture.
m_0 $[M]$ Injected mass
c_0 $[M{\cdot}L^{-3}]$ Constant concentration for a continuous injection
k_B $[M{\cdot}L^2{\cdot}T^{-2}{\cdot}K^{-1}]$ Boltzmann constant
T $[K]$ Absolute temperature
r_p $[L]$ Radius of the solute molecules
τ_c $[T]$ Critical time needed for a particle to experience the whole cross-sectional profile of velocities in a fracture without sorption reaction on the fracture walls
τ'_c $[T]$ Critical time needed for a particle to experience the whole cross-sectional profile of velocities in a fracture with sorption reaction on the fracture walls
x_c $[L]$ Minimum travel distance for which the Taylor–Aris dispersion regime is completely established in a parallel-plate fracture
R_a [−] Retardation factor
$\langle 2b \rangle$ $[L]$ Mean-fracture aperture in a fracture with variable aperture
λ_β $[L]$ Correlation length of the logarithm of the apertures in a fracture with variable aperture
σ_β [−] Standard deviation of the logarithm of the apertures in a fracture with variable aperture
α_g $[L]$ Longitudinal macro-dispersivity in a fracture with variable aperture
h $[L]$ Lag distance (variogram analysis)
P_e [-] Peclet number
$[\phi]_s$ Concentration of the element ϕ in the solid phase, expressed as a mass per unit surface $[M{\cdot}L^{-2}]$ for a sorption on the fracture walls, or as a mass per unit mass of solid $[M{\cdot}M^{-1}]$ for sorption onto the matrix
$[\phi]_{aq}$ $[M{\cdot}L^{-3}]$ Concentration of the element ϕ in the fluid phase
K_d $[L]$ or $[L^3{\cdot}M^{-1}]$ Sorption coefficient
a_w $[L^{-1}]$ Flow-wetted surface
R_f [−] Retardation coefficient (solute sorption on the fracture walls)

$[\varphi]_s^0$ $[M{\cdot}L^{-2}]$ or $[M{\cdot}M^{-1}]$ Maximal concentration adsorbed onto the solid phase
k_{ads} $[L{\cdot}T^{-1}]$ or $[L^3{\cdot}M^{-1}{\cdot}T^{-1}]$ Adsorption rate
k_{dsp} $[T^{-1}]$ Desorption rate
λ $[T^{-1}]$ Decay constant
$t^{1/2}$ $[T]$ Half-life period

c_f^i, c_f^j $[M{\cdot}L^{-3}]$ Aqueous concentration of elements i and j in the fracture (decay chain reaction)

R_f^i, R_f^j [−] Retardation coefficient of elements i and j (decay chain reaction)
ζ_{ij} [−] Fraction of parent element i transformed into element j (decay chain reaction)
M [−] Total number of parent elements i transformed into element j (decay chain reaction)
D_p $[L^2{\cdot}T^{-1}]$ Pore-diffusion coefficient
D_e $[L^2{\cdot}T^{-1}]$ Effective-diffusion coefficient
D_a $[L^2{\cdot}T^{-1}]$ Apparent diffusion coefficient
δ_D [−] Pore constrictivity
τ^2[−] Pore tortuosity
F_f [-] Formation factor
c_m $[M{\cdot}L^{-3}]$ Aqueous-solute concentration in the rock matrix
θ_m [−] Rock-matrix porosity
θ_t [−] Transport porosity of the rock-matrix
θ_s [−] Storage porosity of the rock-matrix
c_s $[M{\cdot}M^{-1}]$ Concentration of the sorbed solute in the solid phase of the rock matrix
D_s $[L^2{\cdot}T^{-1}]$ Diffusion coefficient in the sorbed phase
α [−] Capacity factor including the sorption properties of the matrix
ρ_m $[M{\cdot}L^{-3}]$ Bulk density of the rock matrix
β_F [−] Freundlich exponent
A $[L^2]$ Cross-sectional area of the matrix block normal to the transport direction in the fracture
B $[L]$ Maximal depth of solute penetration in the matrix by diffusion
t'_0 $[T]$ Mean residence time in the fracture
p [£] Laplace parameter

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T^* [T] Half-period of the Fourier series for the numerical inversion of the Laplace transform
E [$M{\cdot}L^{-3}$] Absolute error tolerance for the numerical inversion of the Laplace transform
ρ_c [$M{\cdot}L^{-3}$] Bulk density of the fracture-wall coating
δ_c [L] Thickness of the fracture-wall coating
c_{im} [$M{\cdot}L^{-3}$] Aqueous-solute concentration in the immobile zone (Coats–Smith model)
θ [–] Volumetric fraction of the mobile zone (Coats-Smith model)
θ' [–] Volumetric fraction of the immobile zone (Coats-Smith model)
ω [T^{-1}] Mass-transfer coefficient (Coats-Smith model)
$(c_{im})_j$ [$M{\cdot}L^{-3}$] Aqueous-solute concentration within the j^{th} immobile zone (multiple-rate model)
β_j [–] Ratio of total-solute mass in the immobile zone j, to the mass in the mobile zone at equilibrium (multiple-rate model)
α_j [T^{-1}] Apparent first-order mass-transfer coefficient associated with the j^{th} immobile zone (multiple-rate model)

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