2. LITERATURE REVIEW

During the last 30 years, a great number of researchers have invested their efforts in studying the behaviour of flow and transport in rock fractures (Neretnieks et al., 1982; Moreno et al., 1988; Brown, 1989; Thomson et al., 1991; Cvetkovic et al., 1999; Tsang et al., 2003). This is a consequence of the interest of many countries in finding a proper geological formation in order to store radioactive nuclear waste. For crystalline rocks, the radionuclides are transported mainly through rock fractures. Despite the fact that these studies highlight the application in the storage of nuclear waste, not only are they important for this issue, but also for solving other practical problems that concern the study of flow in rock fractures, such as dam stability and hydraulic fracturing, and flow and transport in rock fractures, such as storage of chemical waste and carbon dioxide storage.

The common assumption to the study of flow in a rock fracture is the assumption that the fracture can be idealised by a pair of parallel plates separated by a constant aperture. In this approximation, the volumetric flow through the fracture is proportional to the cube of the fracture aperture, according to the cubic law, which was reported as valid for deformable rock fractures by Witherspoon et al. (1980). Lately, more realistic descriptions of rock fractures have been reported, considering the roughness of the fractures and the influence that it has on flow properties. A rough fracture take a wide range of aperture values, including contact areas, which leads to a heterogeneous two-dimensional system in which the fluid flow tends to concentrate in certain paths, or channels, of high hydraulic conductivity (see Moreno et al., 1988; Tsang et al., 1989; Abelin et al., 1991b; Hakami, 1996; Lespinasse et al., 2000). Subsequent theoretical (Barton et al., 1985) and experimental studies (Neretnieks et al., 1982) revealed that the parallel plate simplification is not appropriate in describing fluid movement through fractured rocks. The field experiments of large-scale flow and solute migration in the Stripa mine (Abelin et al., 1991a, 1991b) gave evidence that the flow is very unevenly distributed, taking place in individual widely spaced channels in the fractures. Thus, large dry or very low transmissivity areas appear between these channels. A posteriori analysis of this field data was studied by Tsang et al. (1991) using a variable-aperture channel model. Nevertheless, almost all the studies adopt the cubic law as valid locally (Moreno et al., 1988, 1990, 1991; Brown, 1989; Thompson, 1991; Olsson et al., 1993; Cvetkovic et al., 1999; Esaki et al., 1999; Koyama et al., 2005) due mainly to its theoretical simplicity and validity when the fluid velocity is small and the Reynolds number satisfies the laminar flow condition.

2.1. STRESS-FLOW COUPLING IN FRACTURES: EXPERIMENTS AND MODELS

Many coupled stress-flow tests (Tsang, 1990) show the evolution of the flow rate and directional behaviour of the fluid flow under certain stress conditions, usually under normal loading (Gentier, 1987), or combined with shear stress (Esaki et al., 1995b, 1999; Yeo et al., 1998; Lee et al., 2002; Mitani et al., 2002). During these stress processes, the aperture of the fracture changes, and so does the flow. These stress-flow coupling tests were tried to reproduce the phenomena that occur in reality. For instance, the vertical normal stress increases around 0.027 MPa/m with increasing depth, thus changing the void geometry of the fracture. The conductivity of a rock fracture is governed by its complex void geometry that is found between the two surfaces of the fracture, which gives rise to the concept of aperture distribution of the fracture.

The aperture can be defined, as Hakami et al. (1995) suggested, as the distance between the two surfaces of the fracture in the direction perpendicular to a reference plane.
that is assumed to be parallel to the overall fracture surfaces. The aperture is represented by the symbol $b$, and can be characterised by its mean value and its standard deviation. Although Hakami et al. (1990) found that the fracture samples analysed in their study presented a log-normal distribution of the aperture, Hakami et al. (1995) highlighted the fact that there is no consistent evidence that the aperture follows a log-normal distribution, because the experimental data then was still too limited to draw general conclusions. Neretnieks et al. (1982), when comparing the experimental results of the breakthrough curves with the theoretical ones assuming a log-normal distribution of aperture values, found that they did not present a fair resemblance, which means that the channels do not exactly follow a log-normal distribution. Nevertheless, the log-normal distribution is widely adopted (Moreno et al. 1988, 1990, 1991; Tsang et al., 1989, 1990; Wendland et al., 2002).

For the aperture characterization of fractures, another parameter is the correlation length. It gives an idea of how abruptly the aperture changes over the fracture surface area. Fractures with longer correlation length will have contact areas more separated between them, thus creating few channels in which the vast majority of the underground water will flow, as compared to fractures with shorter correlation length. That is to say, for distances in the fracture plane smaller than the correlation length the aperture adopts similar aperture values. With the aid of variograms or correograms, it is possible to quantitatively analyze the correlation length with geostatistical methods (Hakami, 1996). In these diagrams the difference in aperture values of data pairs is presented as a function of the distance between the compared data points, also known as the lag distance.

The aperture of a rock fracture, and consequently its permeability, changes when the state of stress changes. These stress changes can be caused by whether geological activities or human activities, such as underground excavations, man made constructions and blasting (Hakami, 1993). Hakami et al. (1990) reported that the average aperture, together with the spread in aperture values, decreases with increasing normal load. Nevertheless, the ratio between average aperture and standard deviation of the aperture distribution remains almost constant during stress changes (Hakami et al., 1993). An increase in the normal stress value implies that the contact area between the two surfaces of the fracture will become larger and the small apertures will be closed, remaining only the flow channels for conducting flow. Thus, the flowing channelling effect is more obvious under higher values of normal stresses on the fracture. The decrease of flow in the fracture with increasing normal stress was also reported in Gentier (1987). Moreno et al. (1988) reported that the aperture density distribution would be modified when increasing values of normal stress closed the fracture. Recalculating the new log-normal parameters in the new aperture density distribution, it was found that the standard deviation increases with increasing contact area.

In field experiments (Abelin et al., 1991a, 1991b), the hydraulic aperture, which is an equivalent aperture parameter, is calculated from the results of flow tests assuming the validity of the parallel plate model (Hakami, 1996). The hydraulic aperture values are smaller than the mechanical aperture, which is obtained from the arithmetic mean of all the aperture values in the fracture. This is because the flow is concentrated only on a few channels, resulting in a smaller value of the hydraulic aperture with respect to the mean value. The hydraulic aperture values may be considered as the lower limit for the real fracture aperture.

Coupled stress-flow laboratory experiments have been performed by several authors considering different stress conditions, such as normal loading (Gentier, 1987; Lopez et al., 2005), normal and shear loading (Esaki et al., 1995b, 1999; Olsson, 1998; Yeo et al., 1998;
Lee et al., 2002; Mitani et al., 1999, 2002; Jiang et al.; 2004) and rotary shear (Cheon et al., 2002). Figure 2.1 shows the direct shear-flow device with flow parallel to the shear direction used by Mitani et al. (1999), which is a quite standard test. The detail of the sealing mechanism of the shear box can also be seen. Numerical studies considering stress-flow coupling have been done in less occasions (Lespinasse et al. 2000; Koyama et al., 2004, 2005). Recent studies also include the use of Geographic Information System (GIS), which is a powerful tool for visualization, management and analysis of spatial information. A simulation of the compression and flow process in a rock fracture using GIS was conducted by Du et al. (2004), showing an increase in the contact area and a decrease in the aperture values with increasing normal load. Similar results were obtained by Sharifzadeh et al. (2004), but when considering shear displacement, the aperture values increased, indicating unmatching of the fracture’s surfaces due to dilatancy.

Figure 2.1. Schematic diagram of coupled translational shear-unidirectional flow testing device, (a) side view, (b) sealing mechanism of the shear box in 3D and cross section views (Mitani et al., 1999). It should be noted that two normal loading jacks and cells are installed to avoid rotating/tilting of the upper surface during the tests.

A diagram of the coupled translational shear-flow device used by Yeo et al. (1998) can be seen in Figure 2.2. This device allows to reproduce three different kind of flow patterns – radial flow, and unidirectional flow in both directions – by changing flow inlet and outlet, with a shear displacement up to 2 mm. The shear displacement was not continuously applied with no asperity damage produced. It was seen that mean aperture and its standard deviation increased with increasing shear displacement. Apart from this, flow tests showed that with increasing shear displacement, the fracture aperture became more heterogeneous and anisotropic, and permeability in the direction perpendicular to shear displacement was greater than that in the direction parallel to the shear displacement. Similar results were found by Mitani et al. (2002) using a shear-flow coupling device with a radial flow pattern. It was concluded that anisotropy of flow in a rough rock fracture during shear occurs because the contact areas were localized during shear.
Figure 2.2. Schematic diagram of coupled translational shear-flow testing device (Yeo et al., 1998). It should be noted that continuous shear loading cannot be applied in this device. The noticeable feature of this device is both radial and unidirectional flow test conditions can be considered by changing flow inlet and outlet.

Esaki et al. (1999) carried out coupled shear-flow tests with radial flow under constant normal loads and a shear displacement up to 20 mm. It was found that the hydraulic conductivity increased rapidly (with one order of magnitude) for the first 5 mm of shear displacement, but that after this displacement, it reached an almost constant value. Similarly, Lee et al. (2002) found that after 7 or 8 mm shear displacement, the permeability of the fracture gradually reached a threshold value, due to the combined effect of the asperity degradation and the gouge formation. This experiment also contemplated cyclic shear loading, which provoked irregular changes in the fracture permeability, due to the complex interaction between asperity degradation and gouge production.

As for rotary shear, experiments using cylinder specimens have been conducted by some authors (Olsson, 1992; Olsson et al., 1993; Cheon et al., 2002). Cheon et al. (2002) stated that the rotary shear test underestimated the peak shear strength of a rock fracture, because of the varying torque with the radial distance from the axis of rotation. It was found that the mechanical aperture and the hydraulic aperture increased linearly with the increase of the dilatancy. Figure 2.3 shows a schematic view of the coupled stress-flow apparatus used by Cheon et al. (2002), with rotary shear of hollow cylinder specimens with radial flow.
With regards to numerical simulations, Lespinasse et al. (2000) calculated the development of channelling of fluid flows during normal loading, considering an elastic closure of the fracture using a finite difference method. It was found that highly altered fractures presented homogeneous fluxes, although a great number of contact areas appeared during the fracture closure due to normal loading. However, fresh fractures developed strong and increasing flow channels with increasing normal load. The FEM modelling works in Koyama et al. (2004, 2005) did not consider normal load, but translational shear up to 20 mm and rotary shear up to 90 degrees. Shear-induced anisotropy of fluid flow in a single rock fracture under translational shear was reported. A channelling effect in the direction perpendicular to the shear direction produced a predominant flow in this direction. Bidirectional flow patterns, which are more realistic than the common unidirectional shear-flow test that is conducted in the laboratory, were considered, showing that the flow in the direction perpendicular to the shear direction was dominant compared to the flow parallel to the shear direction. For the rotary shear, flow simulations showed that the flow pattern becomes rapidly isotropic with increasing rotary shear angles.

2.2. PARTICLE TRANSPORT PROCESSES IN FRACTURES: EXPERIMENTS AND MODELS

When dealing with particle transport, it is found that there are a number of dispersion mechanisms which elongate an initially steep concentration front in a fracture (Bear, 1988). One is the variation of the random velocities, known as hydrodynamic dispersion. Another one is due to channelling (Bodin et al., 2003). Differences in velocities amongst channels produce a spreading of the front. Furthermore, the transported particles can interact chemically or physically with the surfaces of the fracture, such as sorption reactions, molecular diffusion and matrix diffusion, but they are seldom dealt with in numerical modelling (Cvetkovic, 1991; Cvetkovic et al., 1999; Cheng et al., 2003; Tsang et al., 2003).

With regards to particle transport, two main parameters are of special interest: the mean value and variance of the residence time. The mean residence time in a given channel for non-sorbing tracers (particles) is defined by the volume of the channel over the flow rate
into the channel. These two quantities can be used to determine the dispersion by means of the Peclet number (Pe), which is a dimensionless measure of the dispersivity and is directly proportional to the mean residence time ($\sigma_t$) squared and inversely proportional to the second moment, or variance, of the residence time ($t_w$) of particles in a transport experiment given by the breakthrough curves squared: $2/Pe = \sigma_t^2/t_w^2$. Alternatively, the Peclet number can be estimated from the breakthrough curves knowing the arrival times for $c/c_0$ (ratio of tracer (particles) concentration at the collection point over its initial value at the injection point) equal to 0.1, 0.5 and 0.9 using the following expression: $(t_{0.9} - t_{0.1})/t_{0.5}$ (Neretnieks et al., 1982). Lower values are obtained with this approach, because it detracts importance to the tail. The smaller the Peclet number is, the higher the dispersion is, because it is inversely proportional to dispersion.

Neretnieks et al. (1982) found that the breakthrough curves, which are a plot of the number of particles collected at the end of the fracture at different arrival times, showed a shape with a plateau at about $c/c_0 = 0.8$ for a sample of rock fracture. This shape can be explained by channelling, which is found to be the main dispersion mechanism. The quick channels, with a higher flow rate, carry around 80% of the initial tracer (particles) at the beginning, and afterwards the slower channels eventually will carry the tracers until the breakthrough curves reaches $c = c_0$. As for radionuclides transport Moreno et al. (1988) highlighted that channelling caused a portion of the nuclides to travel at faster speeds than the average speed, giving them less time to decay. Similarly, species interacting with fracture surfaces by sorption or other mechanisms will have less area to react with than if the flow would be equally distributed through all the fracture.

As far as field tracer tests are concerned (Abelin et al., 1991a, 1991b), they are usually carried out by withdrawing water from a borehole, creating a convergent flow field that attracts the tracers, which have been injected at another point, to flow into a sink. Assuming that there is a parallel regional flow in the plane of the fracture, the two opposite sides of the fracture will have a constant hydraulic head difference. For each direction of the pressure gradient, the fluid will seek the least resistive paths. While zones with small aperture values will usually have very little flow, it is possible that zones with large apertures may also not have large flow because they may not be connected to the main flows due to constrictions by the nearby fractures (Tsang et al., 1989). If a tracer is injected in the fracture, it is expected to reach a larger number of paths for larger injection flow. Nevertheless, the pattern of the flow paths is strongly dependent on the aperture distribution near the injection point. In the study carried out by Abelin et al. (1991a, 1991b), evidence was found that flow took place in channels that were not connected between each other. Nevertheless, field experiments are scarce because they are very expensive and require careful preparations. Another drawback is the fact that the fracture distribution and the aperture values of the fractures remain unknown inside the rock mass.

Numerical modelling represents a useful complement to field experiments. Fracture networks have been modelled and studied by several authors (Min, 2004; Öhman, 2005). Although there are different trends in order to quantify flow and transport in fractured networks (Neuman, 2005), it is common to assign a constant aperture value to every fracture. That is to say, the parallel plate model is assumed for every single fracture in the fractured rock mass. Min (2004) studied the effect of stress on the fracture aperture, and found that depending on the state of stress, permeability can decrease or increase with increasing compressive strength, showing the complexity of a fractured network.
In numerical models concerning flow in a single rock fracture, geostatistics are usually used in order to generate a two-dimensional field of a certain distribution of apertures, adopted as log-normal distribution by several authors (Moreno et al., 1988, 1990, 1991; Tsang et al., 1989, 1990; Wendland et al., 2002). This implies that the flow rates can vary several orders of magnitude between two different points, because the log-normal distribution assumes a large range of aperture values, and the cubic law is usually adopted. As for solute transport through the fracture, the particle tracking technique, which consist in following the advected particles through the fracture, is a useful method to model advective processes, such as reported in (Moreno et al., 1988, 1990; Tsang et al., 1989, 2003). With this technique, Moreno et al. (1988) found that the mean residence time of the tracked particles is very similar to the value obtained by dividing the total fracture volume by the total volumetric flow rate through the fracture. A drawback of generating the aperture distribution using geostatistics is that the evolution of the aperture distribution during shearing processes cannot be reproduced readily.

In the work carried out by Moreno et al. (1990), anomalous flow and transport due to fracture aperture variability were dealt with. A square fracture of a grid 40 x 40 is numerically simulated, generated through a log-normal distribution of the aperture and an exponential function for the spatial covariance. Ten fractures with the same aperture density distribution and the spatial correlation length were generated (Moreno et al., 1988). A parallel flow system, with two boundaries opposite to each other with constant pressure value, but one higher than the other, and the other two sides with no-flow condition, was assumed. For the injection of tracers in a parallel flow system, sensitivity studies to determine the minimum number of particles that should be introduced at the injection point in order to obtain reliable results were conducted. They found that in their case, in which the particles were collected at 10 different sections, about 4,000 particles were needed. The results show that the fluid flows through a few main channels, the water flow is concentrated in about 20% of the fracture surface, and flow rates are found to vary by several orders of magnitude. Then, tracers were injected with different water flow rates at different points in the fracture. The local hydraulic conductivity varies over four orders of magnitude, indicating that in a heterogeneous system such as fractures of variable apertures a considerable number of local hydraulic conductivity measurements are needed. It is also found that the correlation length used in the simulations influences the flow distribution strongly. As expected, the larger the injection flow rate is, the higher the residence time and the dispersion are.

To sum up, Moreno et al. (1990) concluded that the hydraulic properties of the fracture, i.e. tracer transport time, mass balance aperture and dispersivity, are influenced by the injection location, the injection flow rate and the channels through which the injected tracers travel. Mainly, there are two possible situations when injecting the tracer. The first one occurs when the tracer is injected in a zone that is directly connected, or almost directly connected, to the collection hole. In this situation, the residence time will be short and the calculated mean aperture may be smaller than the real mean aperture, and the influence of the injection flow rate will be insignificant. The other possible situation is when the injection point is not connected to the collection hole. Here, the tracer spends a long time before entering a main pathway, resulting in a long residence time and in a calculated aperture being very large. Unlike the previous situation, it will be strongly influenced by the injection flow rate. It has to be borne in mind that for a fracture in situ, which is subject to normal stress, it is usually difficult to find direct connection between different points.
Some numerical simulations (Thompson 1991; Thompson et al., 1991; Oliveira et al., 1998; Cvetkovic et al., 1999; Wendland et al., 2002) predict the movement of solute through a rough fracture by solving the advection-dispersion equation (cf. Eq. 11), which give a better description when both advection and molecular diffusion are important. Thompson (1991) stated that the effective velocity of the solute differs from that of the average fluid particle due to transverse and longitudinal dispersion and diffusion, which is in agreement with field measurements of flow and transport in fractures. In addition, Thomson et al. (1991) highlighted that the directional characteristics of the surfaces have a major importance in determining fracture transport properties than has the degree of roughness. Thus, roughness orientated perpendicular to the flow direction decreases flow rates and delays the solute travel time.