1. INTRODUCTION

1.1. BACKGROUND AND MOTIVATION

Disposal of high-level radioactive waste is a paramount worldwide environmental issue today. High-level, long-lived radioactive waste needs to be isolated from the environment for about 100,000 years before its radiotoxicity will have decreased to non-hazardous levels. The most appropriate solution for the disposal of this kind of nuclear waste seems to be repositories placed in stable geological formations deep underground, currently with four main different rock types: crystalline rocks, salt rocks, indurated clays, and plastic clays (Tsang *et al.*, 2005). Figure 1.1 shows an outline of a conceptual underground repository in a stable geological formation.

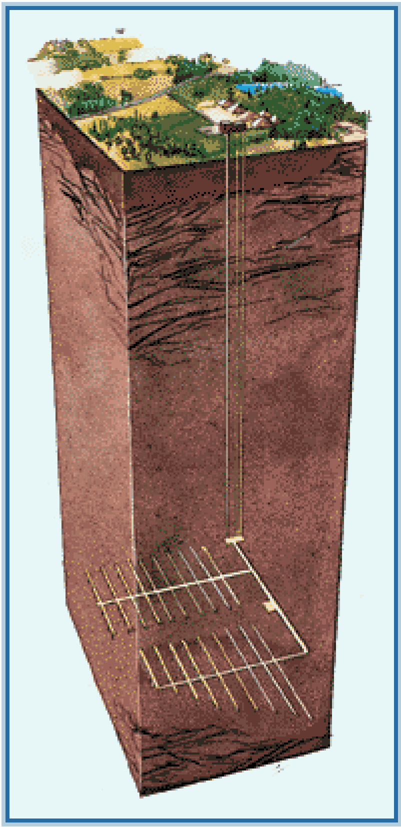

Figure 1.1. Outline of an underground repository in a stable geological formation excavated at a depth of about 500 m (reproduced from STUK, 2004).

No country has started the disposal of high-level radioactive waste yet because there are still many uncertainties about the reliability of underground repositories in preventing radionuclides from reaching the biosphere. In this way, international co-operation is being carried out in order to gain knowledge about the feasibility and long term safety of disposal in stable geological formations deep underground. Figure 1.2 shows a detail of a deposition hole filled with bentonite for an underground repository with natural and engineered barrier systems. The geological formation acts as a natural barrier when the engineered barrier, the bentonite layer and the canister, eventually fail over time.

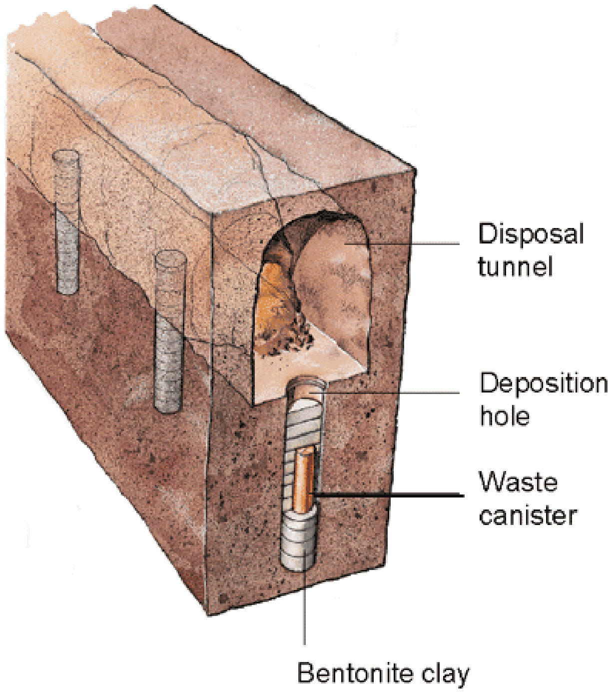

Figure 1.2. Detail of a tunnel with the deposition holes where the canisters are placed and surrounded by bentonite (reproduced from STUK, 2004).

When excavating the disposal tunnels in a fractured rock mass, redistribution of *in situ* stresses occurs and this may provoke significant deformations, such as opening or closing of fractures due to the variations of normal and shear stresses, which will consequently change the flow and transport characteristics of the fractures and the fractured rock masses. The disturbed zone caused by excavation is known as the excavation disturbed zone (EdZ) and/or excavation damaged zone (EDZ), which needs to be studied in detail for the long term safety against leakage of radionuclides once the repository has been closed. It is expected that the rock permeability in the EDZ will increase, especially in the direction parallel to the axis of the tunnel (Kim *et al.*, 2004).

Figure 1.3 shows how a tunnel excavation affects a fractured rock mass with the EDZ shown in pink and the water flowing along fractures (arrows in blue). In this zone, a rearrangement of the stresses may produce shear and opening of fractures. A rough fracture can be idealized as a saw-tooth shaped fracture with an undulation angle α (Jing *et al.*, 1995), as shown in the detail of Figure 1.3. Transmissivity increases anisotropically with shear, being more significant in the direction perpendicular to shear, so that the permeability increases. The flow and consequently the particle transport change as well. During the construction stage, there is flow towards the tunnel, as indicates the blue arrow on the left in Figure 1.3, which hinders the construction of the tunnel. Once the tunnel has been constructed, sustained and sealed, the alteration of the rock properties during the excavation stage increases the natural flow in the direction parallel to the tunnel axis, which can be a problem if a leakage of radionuclides were to occur.

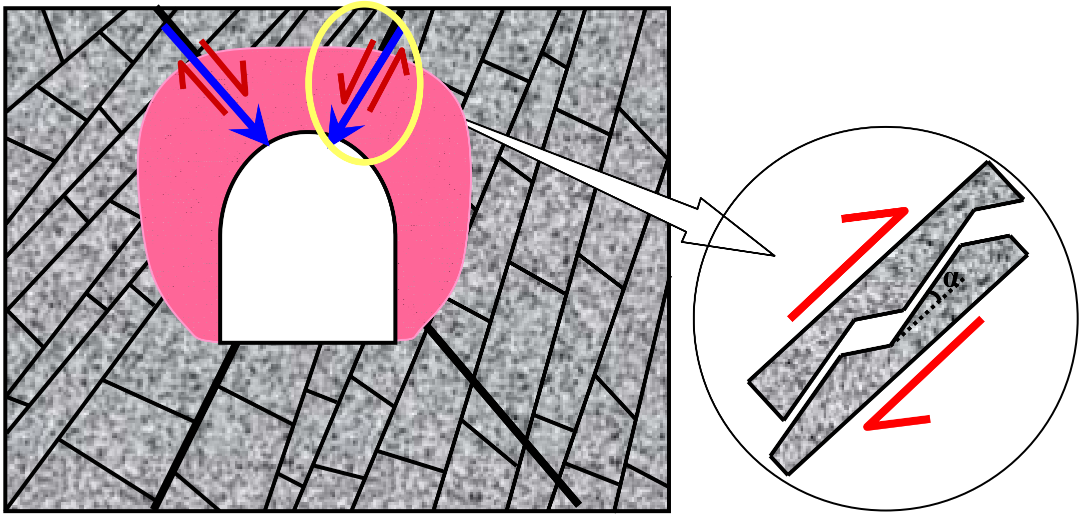

Figure 1.3. Excavation damaged zone (EDZ) and fracture opening due to shear sliding of the fractures when excavating a tunnel in a fractured rock mass.

As far as a single rough rock fracture is concerned, its transmissivity depends on its deformation path and history. It is widely accepted that transmissivity of a single rough fracture decreases with increasing normal stresses, which produces the closure of the fracture (Witherspoon *et al.*, 1980; Gentier, 1987), and that transmissivity increases when shearing processes occur (Barton *et al.*, 1985; Olsson *et al.*, 1993; Gentier *et al.*, 1996). Furthermore, shear-induced anisotropy has been studied by several authors, both at laboratory (Gentier *et al.*, 1996; Yeo *et al.*, 1998) and numerically (Koyama *et al.*, 2005), indicating that the flow perpendicular to shear displacement is predominant over the flow parallel to a translational shear direction.

For laboratory experiments, measuring fluid flowing perpendicular to the shear direction is technically difficult in a linear shear-flow experiment. Despite the fact that coupled stress-flow test with normal and shear loading with unidirectional flow parallel to the shear direction can be measured with high accuracy, coupled stress-flow tests with unidirectional flow perpendicular to shear direction have difficulties in fluid sealing in the direction parallel to the shear direction, especially when large shear displacements are required. An experiment of this kind was performed by Yeo *et al.* (1998), but with only a shear displacement up to 2.0 mm and without carrying out any mechanical direct shear test.

Some coupled stress-flow experiments considering radial flow have been performed using rectangular specimen (Esaki *et al.*, 1995b; 1999; Mitani *et al.*, 2002) and cylinder specimen (Gentier *et al.*, 1996). These experiments helped in evaluating the shear induced flow anisotropy due to the fact that flow can be collected separately in both directions, i.e. parallel and perpendicular to shear direction. Similarly to the experiment mentioned in the previous paragraph, from these studies it was found that flow is predominant in the direction perpendicular to the shear direction.

Numerical modelling experiments for flow and solute transport has been performed by several authors (Neretnieks *et al.*, 1982; Moreno *et al.*, 1988; Tsang *et al.*, 1990; Thompson, 1991; Cvetkovic *et al.*, 1999; Wendland *et al.*, 2002). Most of them used geostatistical methods based on a given aperture probability density distribution and a specific spatial correlation length to generate the aperture distributions, and concluded that due to the roughness of the fracture fluid flows following some dominant paths or channels, which offer the least resistance. Some models are quite sophisticated, considering matrix diffusion (Cvetkovic, 1991; Kennedy *et al*., 1995). Nevertheless, these models did not take the effects of shearing processes into account.

In the present study, a numerical modelling of fluid flow and particle transport in a single rough fracture during shear is conducted. The study focuses on the effects of different boundary conditions (some of which cannot be performed satisfactorily in the laboratory, e.g. unidirectional flow perpendicular to shear direction) and the combination of shearing processes with fluid flow and particle transport, which has not been performed before. This research will, therefore, represent a challenging opportunity to obtain some new findings in the field of coupled hydro-mechanical behaviour of flow and particle transport in a rough fracture. Figure 1.4 shows the coupled hydro-mechanical process considered in the current study, and its relation to particle transport.

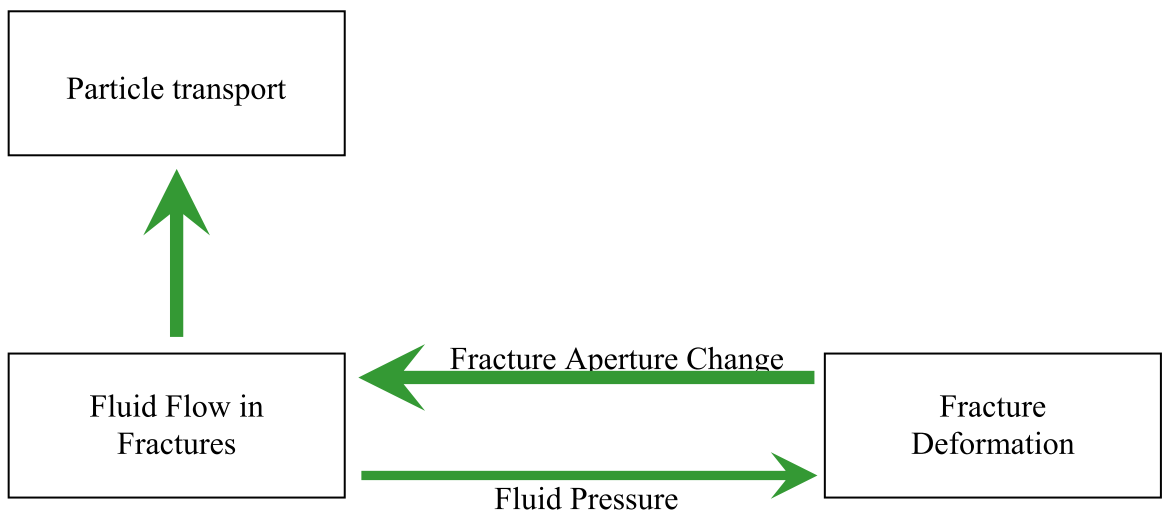

Figure 1.4. Coupled H-M process in fractures and its relation with particle transport.

1.2. OBJECTIVES

The overall objective of this thesis is to address coupled fluid flow and particle transport in a single rough fracture during shear. A first step towards achieving this objective is to characterize the roughness of the fracture, by means of analysing the evolutions of the aperture and the transmissivity fields during shear, using geostatistical tools. Thus, differences in the transmissivity along different directions in the fracture can be identified, and therefore possible anisotropy in fluid flow can be determined. Particle tracking in the fracture is then carried out using the fluid velocity fields calculated with a Finite Element Method (FEM) code. The aim of this modelling is to gain knowledge about how shear processes affect particle transport in a rough fracture. Different boundary conditions were considered, having special interest those that cannot be reliably reproduced in the laboratory tests, such as unidirectional flow perpendicular to shear direction and bi-directional flow patterns.

In the following chapters, first a literature review is presented concerning both experiments and numerical modelling of stress-flow coupling in rock fractures, together with a summary of the particle transport experiments and numerical simulation (Chapter 2). Next, the methodology used for this research is explained in detail, including sample preparation and aperture representation, characterization of surface roughness using semi-variograms, and the numerical methods for both the FEM code used for flow calculation and the code that was developed for the particle tracking (Chapter 3). The results and discussions are presented (Chapter 4). The studied issues are divided into two main topics, which are the characterization of roughness, aperture and transmissivity fields using semi-variograms, in both translational and rotary shear processes, and coupled fluid flow and particle transport during shear with different flow patterns, such as unidirectional flow patterns with flow parallel and perpendicular to shear direction, bi-directional flow pattern and radial flow patterns, considering translational and rotary shear. Conclusions are drawn (Chapter 5). Finally, some recommendations for future research are stated (Chapter 6).