

ABSTRACT

Title: Numerical Modelling of Fluid Flow and Particle Transport in a Rough Rock Fracture during Shear

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Disposal of high-level radioactive waste is a crucial worldwide environmental issue today. The most appropriate solution for the disposal of this kind of nuclear waste seems to be repositories placed in stable geological formations deep underground. 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. Numerical modelling for flow and solute transport performed up to date mainly use geostatistical methods based on a given aperture probability density distribution and a specific spatial correlation length to generate the aperture distributions, reporting that due to the roughness of the fracture fluid flows following some dominant paths or channels, which offer the least resistance, without considering the shear effects. This 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 an opportunity to obtain some new findings in the field of coupled hydro-mechanical behaviour of flow and particle transport in a rough fracture.

The effects of both translational and rotary shear on particle transport under coupled shear-flow test conditions in a single rough rock fracture were numerically investigated in this thesis. A pair of digitalized surfaces of a 250x250 mm concrete rough fracture replica was numerically manipulated to simulate the translational and rotary shearing processes of the sample without considering normal loading and asperity damage, using Finite Element Method (FEM). From the evolutions of the aperture distributions during the shearing processes the evolutions of the fracture transmissivity fields were determined. Different fluid flow situations were considered. For the translational shear, with 1 mm shear displacement interval up to 20 mm, three different flow patterns - unidirectional (flow parallel and perpendicular to the shear direction), bi-directional and radial - have been taken into account. For rotary shear, with a 0.5° shear angle interval up to 10°, only the radial flow pattern has been taken into consideration. Furthermore, the effect of the fracture surface roughness on the aperture and transmissivity fields was evaluated using semi-variograms.

The results from the geostatistical approach show that translational shear generates a significant channelling effect perpendicular to the shear direction, which provokes a shear-induced anisotropy in the aperture and transmissivity distributions. Rotary shear induces an isotropic transmissivity field with high correlation in all directions. The results of flow and particle transport simulations show that shearing processes make rough fractures much more permeable, producing a significant decrease in travel time of the particles, especially at the start of the shear processes. Translational shear yields a channelling effect in the direction perpendicular to the shear direction, creating high transmissivity channels through which particles travelling in this direction can travel fast and without being delayed by bypassing low transmissivity areas, as it happens when the fluid flows parallel with shear direction. Bi-directional flow patterns show clearly the shortcomings of the conventional shear-flow tests in the laboratory with a unidirectional flow. In radial flow patterns, while translational shear generates an anisotropic particle transport behaviour with faster transport perpendicular to the shear direction, rotary shear presents isotropic flow field and particle paths in all directions. The studied flow and particle transport simulations provide a first step towards a better understanding of particle transport in coupled stress-flow processes.