DEM study of the mechanical behavior of a leached interface upon shearing

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ABSTRACT: It has been shown that contacts between host rock and engineered barriers may be critical in the design of deep radioactive waste repositories. Water is expected to reach the interface zone after the re-saturation of the geological massive and its presence may lead to concrete leaching. Such a phenomenon could increase the interface transmissivity and compromise the confinement of radioactive waste. Recent experimental results from Buzzi et al. (2008) have enhanced how concrete leaching can drastically change the mechanical behaviour of such interfaces. Because of the local loss of strength resulting from leaching, shearing resulted in a degradation of the interface asperities. Similarly to rock joints, intact interfaces exhibit a usual contracting-dilating behaviour. On the contrary, depending on the extent of leaching, the degraded interface can display a fully contracting. This paper intends to investigate the influence of concrete leaching on the mechanical behaviour of host rock-concrete interfaces. The leaching process consists in the dissolution of some of the hydrates of the cement paste, leading to a reduction of the strength and Young's modulus. A discrete model has been developed with PFC3D where a simplified interface morphology has been introduced using a saw-tooth description of the asperities.

1 INTRODUCTION

Many nations such as France, Canada, Japan or Spain to name a few, are currently facing the issue of nuclear waste storage. Comprehensive studies have been performed to better understand the materials involved in the design of both engineered and natural barriers (rock, concrete or bentonite in various forms) and their possible interactions (Gens et al., 2002; Grindrod et al., 1999). Considering the very long service life required for the engineered barrier, some studies are devoted to long term behaviour of materials with an emphasis on aging or degradation. One of the possible degradation phenomena is calcium leaching, which generally affects cementitious materials in presence of water. During this process, several chemical components of the cement paste such as portlandite are dissolved, resulting in a local increase of porosity. Calcium leaching has mainly been studied in laboratory using accelerated kinetics (by ammonium nitrate (Carde, 1996) or by electrical potential (Saito and Deguchi, 2000)) and it is now quite well understood. Natural leaching is a very long process and very few data are available in the literature about long term degradation of concrete by pure water (e.g. Tragardh et al., 1998). Experimental studies performed on cementitious materials and structures have shown that leaching induces a mechanical weakening. The degraded material experiences a loss of mechanical strength and a reduction of stiffness (Le Bellego et al., 2000; Gerard, 1996; Carde, 1996).

To date, the transfer properties of leached cementitious materials (e.g. permeability) have not been widely investigated as they are usually correlated to the porosity by means of empirical formula (Ollivier and Massat, 1992; Luping and Nilsson, 1992). So far, most of the conclusions about the effects of leaching were drawn from tests performed on bulk materials. Little data are available on the impact of leaching on interface despite their importance for the efficiency of the nuclear waste repository (Dixon et al., 2002). A recent experimental study by Buzzi et al. (2008) has shown that, as expected, a leached interface exhibits a lower shear strength than an intact interface. The authors have also observed a decrease of transmissivity followed by a large increase when the aggregates are pulled out of the specimen.

This paper aims to complement the experimental study after Buzzi et al. (2008) by means of a numerical model. The distinct element code PFC3D has been used to simulate constant normal shear tests on intact and leached interfaces. The method to implement the leaching has firstly been validated by means of unconfined compression tests. Then, a simple saw tooth geometry has been tested under different levels of constant normal stress. Several leaching depths have been implemented in the interface to identify more precisely the effect of leaching on the mechanical response upon shearing. The results tend to corroborate the conclusions obtained by Buzzi et al. (2008).

2 CALIBRATION OF INTACT AND LEACHED MATERIAL

2.1 *Intact mortar*

Distinct Element Method inherently offers the possibility to capture the increase of macroporosity resulting from leaching and the breakage of contact asperities, two key phenomena of the present problem. Consequently, a DEM code has been used, namely PFC3D from Itasca (Potyondy and Cundall, 2004). In this method, a body is described by rigid particles, which interact according to contact laws and micro-properties. The calibration of these latter follows the procedure described by Potyondy and Cundall (2004) and usually aims to reproduce given macro properties. Herein, numerical unconfined compression tests on cylindrical specimens were performed and comparison was made between experimental and numerical values of Young's modulus and unconfined compressive strength (UCS). The leached material considered in the present work is the mortar tested by Bernard et al. (2008) and by Le Bellego et al. (2000). Significant experimental data are available on this mortar.

To be consistent with a description of mortar, two kinds of particle have been considered in the DEM mortar specimen: cement and sand. Considering a volumetric air fraction of 3% in the mortar (Bernard et al., 2008), its composition (1380 kg/m^3 of sand) and assuming G_s=2.65 for the sand, it can be deduced that 46% of the particles of the numerical sample represent cement and 54% represent sand. These particles are distributed randomly in the specimen. The sand and cement particles have the same density but different stiffness. As suggested by Bernard et al. (2008), the stiffness of the sand-sand contact is approximately 3.5 times greater than the stiffness of the cement-cement contact. Note that an equivalent stiffness is automatically considered by PFC3D for the cement-sand contact. For each particle type, the bond normal and shear stiffness are equal to the corresponding particle contact stiffness. The bond strength of the sand-sand contact and cement-cement contact are the same for a matter of simplicity. The set of material parameters and the resulting macroscopic mechanical properties are presented in Tables 1 and 2, respectively.

Table 1. Material parameters for intact contact.

Description	Cement	Sand
Particle properties		
Particle contact modulus [GPa]	18.0	63.0
Ratio of particle normal to shear stiffness (kn/ ks)	2.5	2.5
Particle friction coefficient	0.364	0.364
Parallel-bond properties		
Parallel-bond radius multiplier	1.0	1.0
Parallel-bond modulus [GPa]	18.0	63.0
Ratio of parallel-bond normal to shear stiffness	2.5	2.5
Mean value of bond normal strength [MPa]	69.5	69.5
Standard deviation of bond normal strength [MPa]	5	5
Mean value of bond shear strength [MPa]	69.5	69.5
Standard deviation of bond shear strength [MPa]	5	5

Table 2. Results of the calibration for the intact mortar.

Properties	Experimental	Numerical
UCS [MPa]	68.1	62.3
E [GPa]	44.1	44.6

2.2 *Leached mortar*

Leaching of cement paste leads to increase of macroporosity due to the dissolution of chemical components, namely Calcium Silicate Hydrates (CSH), Calcium Hydroxides (CH) and Hydrated Aluminates (HA). The consequence of this increase of macroporosity is a reduction of mechanical properties (Carde, 1996). Similarly, here the mechanical properties of the material are not diminished; only the macro porosity is progressively augmented with leaching. Extensive studies on leaching have shown the existence of several dissolution fronts. Carde et al. (1999) and Bernard et al. (2008) have identified four leached zones of different chemical composition in their study (see Figure 1). Their results were used to implement similar leaching process in terms of front position and amount of species dissolved.

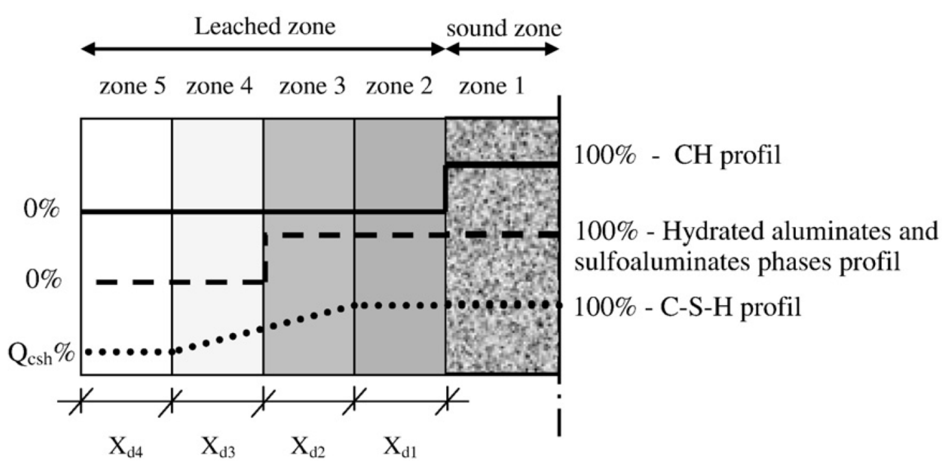

Figure 1: Different leached zones and their composition after Bernard et al. (2008).

Data at 28, 56 and 98 days of leaching are used to estimate the chemical composition of each zone and the position of the dissolution fronts at any leaching depth (Figure 2(a) and (b)). Note that in terms of chemical composition, the amount of CSH in zones 3, 4 and 5 varies with leaching time (Figure 1). The amount of CSH in a given zone, is progressively reduced when leaching time (and thus depth) increases whereas fraction of CH and HA is either 0% or 100%. These data (front positions and chemical compositions) are used to numerically increase the local porosity for any leaching depth. To do so, it is assumed that CSH, CH and HA have the same properties (density, mechanical properties, size distribution) and are distributed randomly in the specimen.

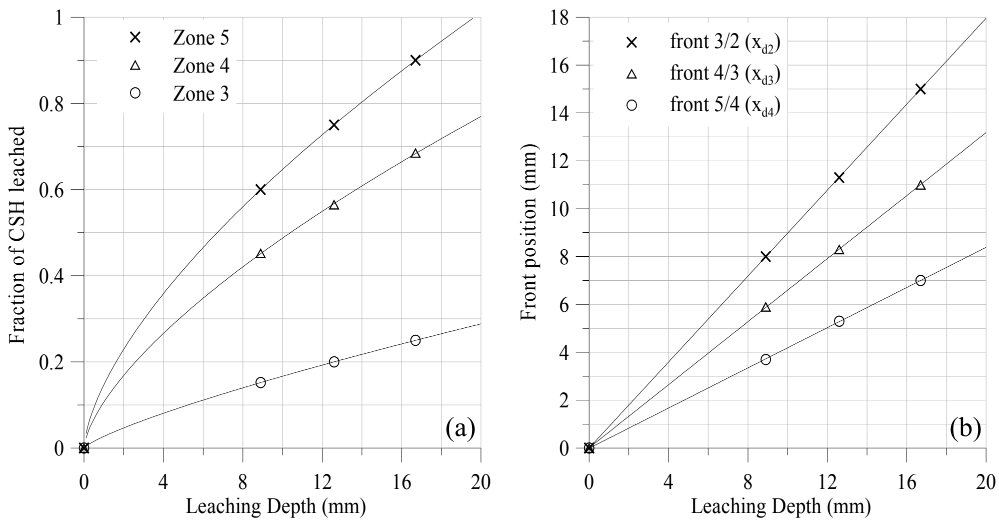

Figure 2: (a) Evolution of fraction of leached CSH with respect to leaching depth. (b) Position of leaching fronts with respect to leaching depth. Symbols correspond to experimental data, lines are curve fitting: power in (a) and linear in (b).

The increase of porosity is implemented as follows:

- As explained before, cement particles represent 46% in volume of the mortar. The volumetric proportions of CH, CSH and HA in the cement paste are known (14.7%, 40.2% and 17.9%, respectively after Bernard et al., 2008). Consequently, CH, CSH and HA represent 8.2%, 22.4% and 10% in volume of the numerical specimen.
- For any leaching depth, the position of the different dissolution fronts is estimated using Figure 2(b).
- In each zone, the fraction of particles to be dissolved can be estimated using Figure 1 and Figure 2(a).
- The total percentage of particles to be removed in each zone is the sum of the fraction to be dissolved for each component.

For example, considering a total leaching depth of 10 mm, it can be estimated that:

- x_{d2} = 9 mm, x_{d3} = 6.6 mm, x_{d4} = 4.2 mm,
- All CH are removed from zones 2 to 5, which represents 8.2% in volume of the total number of particles in the numerical specimen
- All HA are removed from zones 4 and 5, which represents 10.0% in volume of the total number of particles in the numerical specimen
- 65% of CSH are to be removed from zone 5, 49% from zone 4 and 17% from zone 3. This represents respectively 14.5%, 10.9% and 3.7% of the total number of particles in the numerical specimen.
- In conclusion, 32.7% of the particles will be removed in zone 5, 29.1% in zone 4, 11.9% in zone 3, 8.2% in zone 2 and none in zone 1.

3 VALIDATION OF THE INCREASE OF POROSITY DUE TO LEACHING

The method to implement the leaching process has been validated via some unconfined compression tests on cylindrical specimens (see Figure 3). The decrease of Young's modulus and of unconfined compressive strength with leaching time have been compared to experimental data after Bernard et al. (2008) and Le Bellego et al. (2000) in Figure 4. A relatively good agreement is found between experimental and numerical data, thus validating the implementation of leaching.

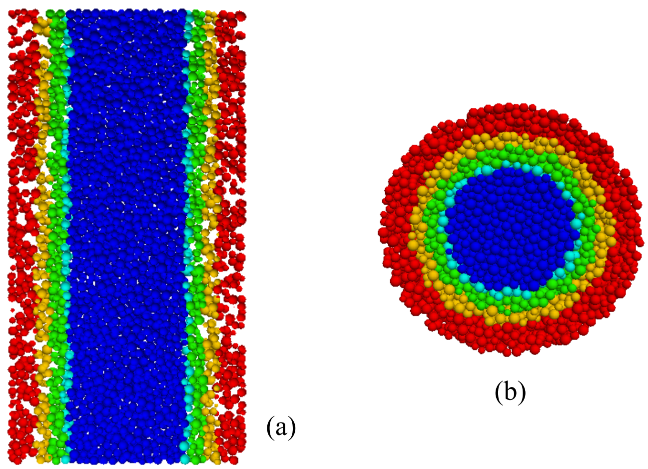

Figure 3: View of the cross slice (a) and longitudinal section (b) of specimen leached for 98 days and subjected to unconfined compression test (diameter 70 mm, height 140 mm). Blue material is sound (zone 1 at the center); red material is the most degraded (zone 5 in periphery).

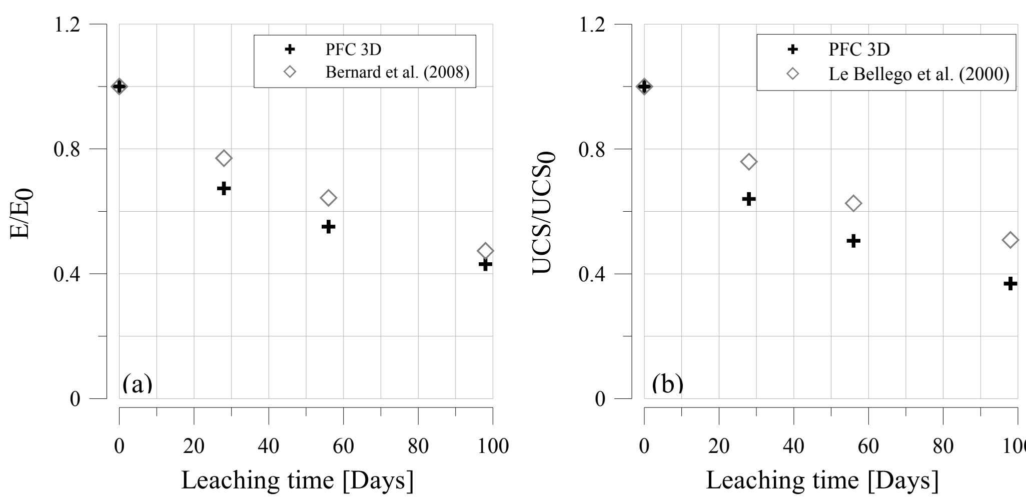

Figure 4: Validation of the implementation of leaching: (a) Evolution of ratio of Young's modulus over initial Young's modulus. (b) Evolution of ratio of unconfined compressive strength over initial unconfined compressive strength.

3.1 *Intact interface*

The effect of the leaching of a rock concrete interface is firstly assessed on an idealized geometry, for which the typical behavior is known. The saw tooth interface (angle of 30°, height of 5 mm) studied by Yang and Chiang (2000) has been modeled using PFC3D (Figure 5). The rock-mortar specimen is built on 33200 particles having a diameter ranging from 0.7 mm (in the vicinity of the interface) to 3.7 mm. The interface is frictional (friction angle of 20°) and the recent "Smooth Joint Model" (SJM) function (Mas Ivars et al., 2008) enables an accurate description of the frictional / dilational behaviour of the interface independently of the size of the particles. The mechanical contact properties are those defined in section 2.1. The specimen is firstly subjected to a compression along axis y (Figure 5) and then to a shearing along axis x at constant normal stress. Displacements along z are restrained. The sum of contact forces on the periphery of the upper half are used to compute the normal stress and shear stress.

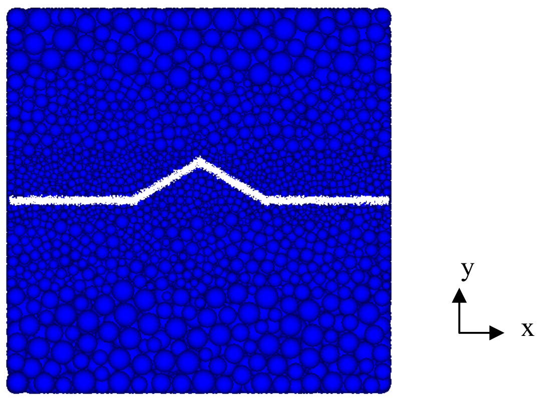

Figure 5: View of the joint model using DEM code PFC. Dimensions of the model: 50 mm (X) × 50 mm (Y) × 40 mm (Z). The contact plane is represented in white.

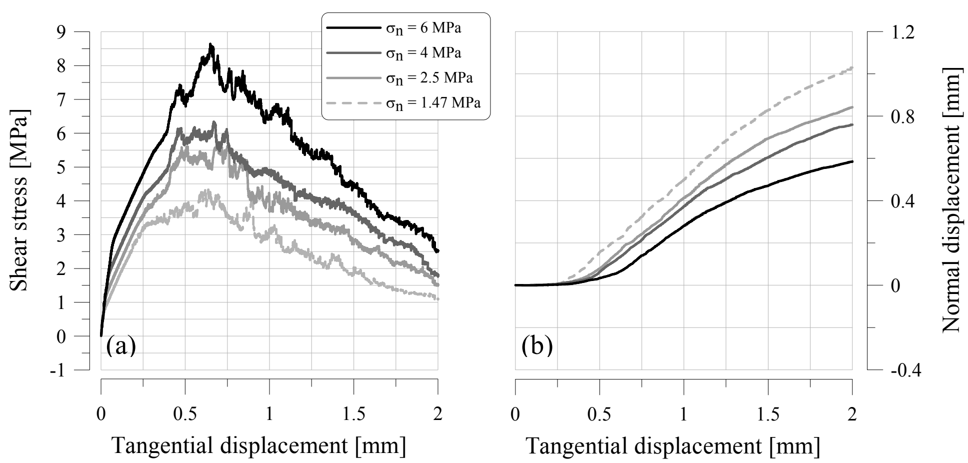

Figure 6: Numerical results on intact interface. Evolution of: normal displacement vs. tangential displacement, (b) Shear stress vs. tangential displacement for different level of normal stress.

The classical mechanical behaviour of rock joints is exhibited in Figures 6(a) and 6(b). The evolution of shear stress with tangential displacement and normal stress follows the usual pattern: the higher the normal stress, the higher the shear stress. Also, the peak in stress occurs in the first 2 mm of shearing. Again, the initial slight contraction of the joint is followed by a significant dilation, the magnitude of which is a function of the level of normal stress. These numerical tests are useful to validate the qualitative behaviour of the intact interface. Should any change take place for the leached interface, they will be imputed to the leaching process.

3.2 *Leached interface*

Rock and mortar constituting the degraded interface have the same mechanical properties than previously. The porosity of the mortar is augmented to reproduce the degradation phenomenon. Leaching is due to the presence of water in the interface and dissolution fronts progress perpendicularly to the contact plane, creating the zones shown in Figure 7. In the following, depth will be preferred to time to quantify the amount of leaching.

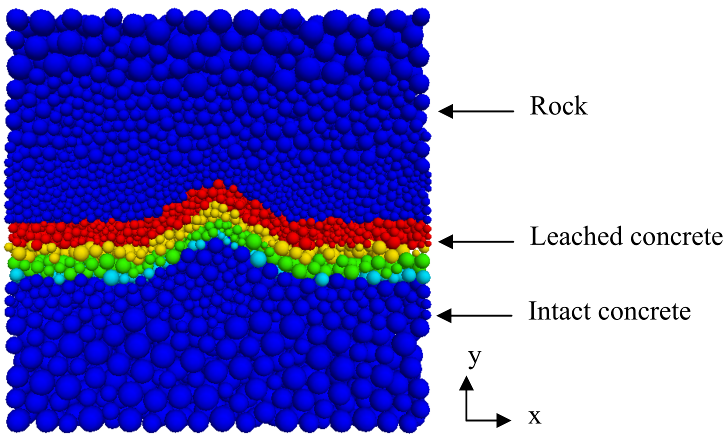

Figure 7: View of the joint model using DEM code PFC. Dimensions of the model: 50 mm (X) × 50 mm (Y) × 40 mm (Z). View of the leached zones in the lower half of the contact. Leaching Depth (LD) of 7 mm.

It is clear from Figures 8 (a) and (b) that the mechanical response of the interface is significantly affected by the leaching depth. Firstly, the shear strength of the interface significantly drops when the leaching depth increases. Two distinct phases take place during this mechanical weakening. Until a leaching depth of 5 mm, a part of the tooth is still intact creating a hard point in the contact, through which forces are still transmitted (see Figure 9(a) and 9(b)). The most significant loss of strength takes place during this first phase (around 50%) and can be explained by the weakening of the bulk material (Carde, 1996; Le Bellego et al., 2000**).** After 5 mm of leaching the tooth is totally weakened and there is no hard point in the contact. It can be seen from Figure 9(c) that the transmission of forces within the contact is more uniform. For more extended leaching, the shear strength keeps decreasing but at a slower rate. This is explained by the fact that the amount of CSH in zone 5 is not constant and the porosity in this zone increases with the leaching depth inducing a lower resistance.

Another remarkable feature of the behaviour of the leached interface is that dilation progressively vanishes so that the joint becomes fully contractant. The change of behavior from contraction/dilation to full contraction is due to the fact that a compaction band develops in zone 5, which is the most porous. As expected the deeper the leaching front, the wider the compaction band and consequently, the more the interface will contract. This is a crucial result for the hydro-mechanical behaviour of the leached interface. Indeed, a contraction of the interface will result in a reduction of its transmissivity. This has been observed experimentally (e.g. in Hans and Boulon, 2003) and it is also suggested by the Reynolds equation (Yeo et al., 1998) or by the cubic law (Zimmerman and Yeo, 2000). All these results are consistent with the conclusions drawn by Buzzi et al. (2008).

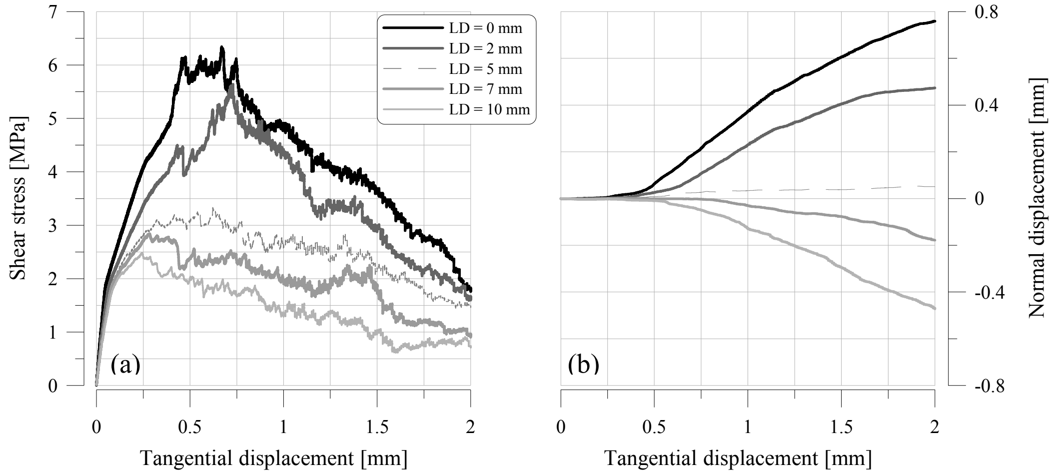

Figure 8: (a) Evolution of shear stress versus tangential displacement. (b) Evolution of normal displacement versus tangential displacement. Shear test under constant normal stress of 4MPa. Leaching depth ranges from 0 mm to 10 mm.

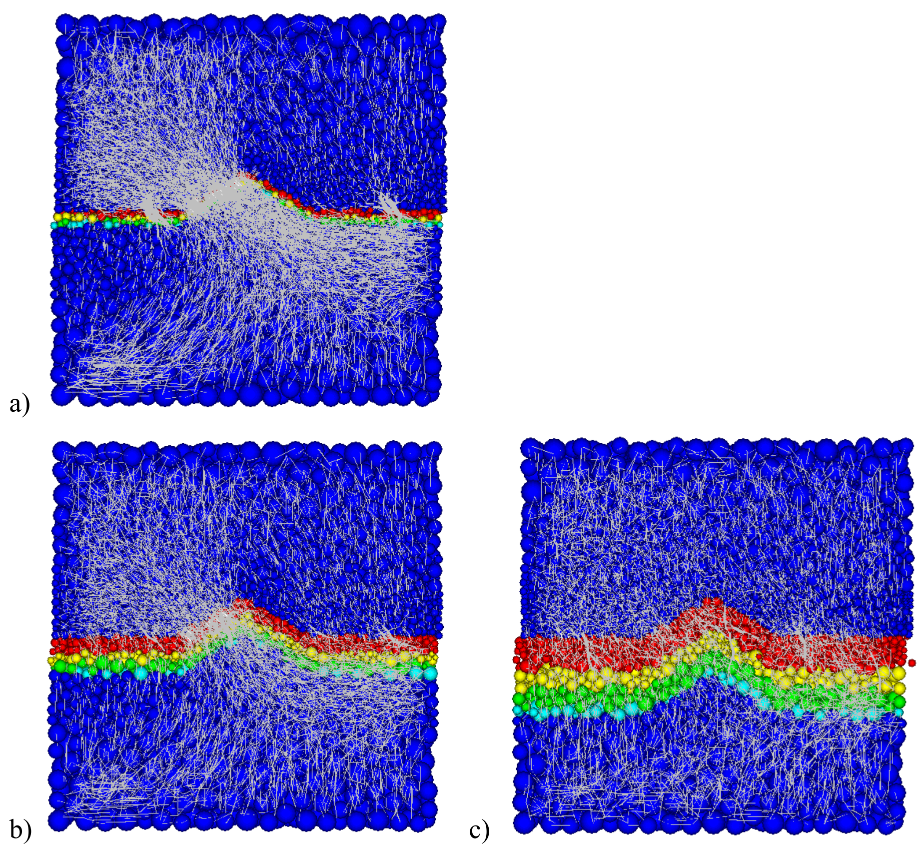

Figure 9: View of the chain forces after 0.6 mm shear displacement for different leaching depth: 2mm (a), 5mm (b) and 10mm (c). Thickness of the line represents the intensity of the contact force.

Numerical shear tests under increasing normal stress were performed in order to determine the failure criterion of the various conditions of interface. Results are plotted in Figure 10 where the approximate Mohr Coulomb criteria are estimated. Again, the two stage loss of mechanical strength is visible. First both friction angle and cohesion decrease significantly. The friction angle of material drops from around 40^o for an intact interface to around 20^o for the leached interface, which corresponds to the friction angle of the interface. Then, after 5 mm of leaching, the interface only experiences a slight loss of cohesion.

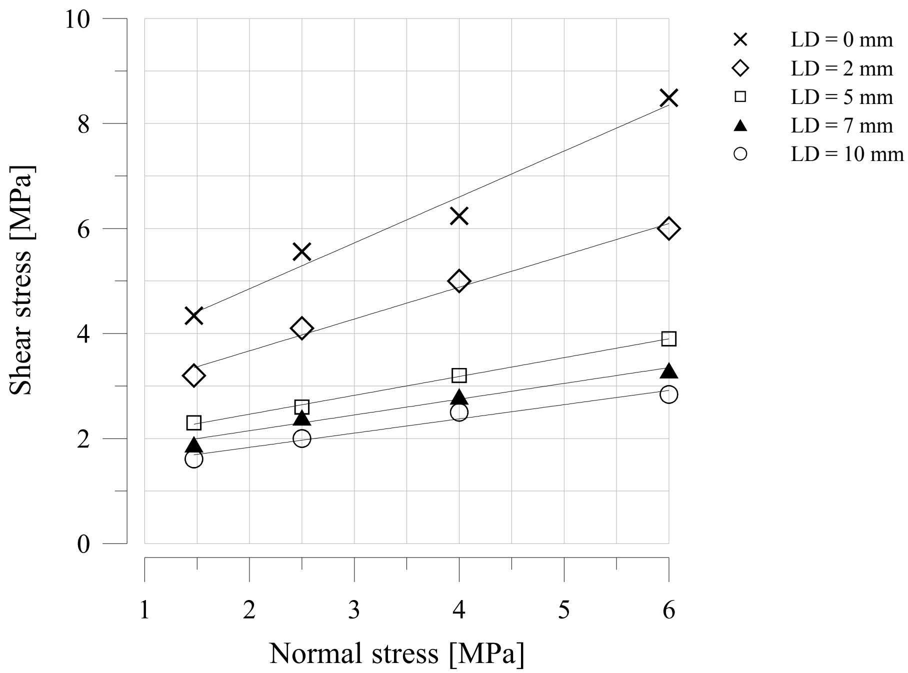

Figure 10: Failure criterion of intact and leached interfaces.

4 CONCLUSIONS AND PERSPECTIVES

Calcium leaching is a long term degradation phenomenon of cementitious materials in presence of water. Experimental studies have shown that leaching induces a local increase of porosity in the bulk material due to the dissolution of several components of the hardened cement paste. As a result, the degraded material experiences a loss of mechanical strength and a reduction in Young's modulus. So far, attention was focused on bulk material and very little data is available on the mechanical behaviour of leached interfaces. Interfaces are nonetheless crucial for the efficiency of deep nuclear waste repository. In this paper, a distinct element numerical model was built to implement the leaching and to test a simple saw tooth interface to shear tests under constant normal stress. The results show that leaching clearly affects the mechanical response of the interface with a progressive loss of shear strength and a change of behaviour from brittle to ductile. Another remarkable feature is the disappearance of dilation. After a sufficient exposure to leaching, the joint becomes fully contractant. This is a crucial result for nuclear waste problem as a contraction will very likely result in a reduction of the transmissivity of the interface.

The next step of this research is to model a natural joint morphology in order to work with a more realistic roughness and to check the validity of the present results. Also, it is expected to produce a hydro-mechanical coupling to evaluate the influence of leaching on the transmissivity of the interface.

5 REFERENCES

Bernard, F., Kamali-Bernard & S., Prince, W. 2008. 3d multi-scale modelling of mechanical behaviour of sound and leached mortar. *Cement and Concrete Research*, 38:449–458.

Buzzi O., Boulon M., Hervé M. & Su.K. 2008 Leaching of rock concrete interfaces. *Rock. Mech. & Rock Eng,* 41(3): 445-466.

Carde, C. & Francois, R. 1999. Modelling the loss of strength and porosity increase due to the leaching of cement pastes. *Cement and concrete composites*, 21:181–188.

Carde, C., Francois, R. & Torrenti, J. M. 1996. Leaching of both calcium hydroxide and csh from cement paste: modelling the mechanical behaviour. *Cement and concrete research*, 26(8):1257– 1268.

Dixon, D. A., Martino, J. B., Chandler, A., Sugita, Y. & Vignal, B. 2002: Water uptake by a clay bulkhead installed in the tunnel sealing experiment at atomic energy of Canada's underground research laboratory. In*: Clays in natural and engineered barriers for radioactive waste*
confinement. Experiments in underground laboratories, Reims, ANDRA.

Gerard, B. 1996. Contribution of the mechanical, chemical and transport couplings in the long term behavior of radioactive waste repository structures. Ph.D. thesis, Laval University, Quebec, Canada - Ecole Normale Superieure de Cachan, France.

Gens, A., Guimaraes do N. L., Garcia-Molina, A. & Alonso, E. E. 2002: Factors controlling
rock-clay buffer interaction in a radioactive waste repository. *Engineering Geology* 64, 297–308.

Grindrod, P., Peletier, M. & Takase, H. 1999: Mechanical interaction between swelling compacted clay and fractured rock, and the leaching of clay colloids. *Engineering Geology* 54, 159–165.

Itasca Consulting Group (2005): PFC3D version 3.1. *User Manual*.

Hans, J. & Boulon, M. 2003: A new device for investigating the hydromecanical properties of rock joints. *Int. J. Numer. Anal. Meth. Geomech*. 27, 513–548.

Le Bellego, C., Gerard, B. & Pijaudier-Cabot, G. 2000. Chemo mechanical effects in mortar beams subjected to water hydrolysis. *Journal of Engineering Mechanics*, 126(3):266–272.

Luping, T. & Nilsson, L. O. 1992. A study of the quantitative relationship between permeability and pore size distribution of hardened cement paste. *Cement and Concrete Research*, 2:542–550.

Mas Ivars, D., Potyondy, D., Pierce, M., & Cundall, P. 2008. The smooth joint contact model. In *Proceedings of the 8th World Congress on Computational Mechanics*. Venice, Italy, paper 2735

Ollivier, J. P. & Massat, M. 1992. Permeability and microstructure of a concrete: a review of modelling. *Cement and Concrete Research*, 22:503–514.

Potyondy, D. O. & Cundall, P. A. 2004. A bonded-particle model for rock. *International Journal of Rock Mechanics and Mining Science*, 41:1329–1364.

Saito, H. & Deguchi, A. 2000. Leaching tests on different mortars using accelerated electrochemical method. *Cement and Concrete Research*, 30:1815–1825.

Tragardh, J. & Lagerblad, B. 1998. Leaching of 90-year old concrete mortar in contact with stagnant water. *SKB*, TR-98-11.

Yang, Z. H. & Chiang, D. Y. 2000. An experimental study on the progressive shear behavior of rock joints with tooth-shaped asperities. *International Journal of Rock Mechanics & Mining Sciences*, 37:1247–1259.

Yeo, I.W., De Freitas, M.H., Zimmerman, R.W. 1998. Effect of shear displacement on the aperture and permeability of a rock fracture. *International Journal of Rock Mechanics & Mining Sciences*;35(8):1051–70.

Zimmerman, R.W. & Yeo, I.W. 2000. Fluid flow in rock fractures: from the Navier–Stokes equations to the cubic law. In: Dynamics of fluids in fractured rock, geophysical monograph 122, American Geophysics Union, Washington, p. 213–24.