Abstract
The mechanical behavior of ordinary Portland cement paste is represented using a numerical model based on the finite element method, with the distinctive features of representing explicitly the first-level heterogeneities and using fracture-based zero-thickness interface elements to model cracks. The model, previously applied to micromechanical analysis of heterogeneous materials such as concrete or mortar, is used to analyze a micro-indentation test with spherical indenter. Preliminary results in 2D have been obtained for cement paste images reported by NIST, from which a first geometric representation in two phases has been developed. The results obtained show the development of the cracks with the indenter penetration, with reasonable failure patterns and load-displacement curves, while at the same time (and with the same parameters) also representing adequately compression and tension failures. These results are considered very promising in the context of an on-going research line aimed at using numerical models in combination with indentation tests, in order to characterize not only elasticity but also strength and fracture-based parameters of cementitious materials in the small scale.

1. INTRODUCTION
In recent years, research focus has shifted toward lower scales of observation in cementitious materials, since it is becoming clear that it is only at those scales that some crucial aspects of durability processes can be understood and modified for design purposes. Cracking of cement paste at the small scale may have dramatic influence no only on the mechanical behavior itself, but also on transport properties which are crucial for the development of durability phenomena. Measuring and characterizing cracking at the small scale, however, poses a real challenge since at that scale it is not easy (and in general not possible) to conduct standard mechanical tests including fracture tests. Perhaps the only mechanical tests nowadays available at the small scale are indentation tests [1-2]. In particular, nano-indentation with sharp indenters is being used more often to characterize the individual basic building blocks of cement paste, namely the two kinds of CSH, portlandite...
and remaining unhydrated clinker particles, while micro-indentation with sharp or blunt indenter has been advocated to get additional information on the overall behavior of the cement paste including also the interaction effects between components and their interfaces.

However, interpretation of those tests for cement paste is not straightforward due once more to cracking. One possible solution consists of using advanced numerical models and perform inverse analysis on a range of sizes/scales and indentation forces.

As a first step in this direction, the authors have adapted an existing meso-level numerical model originally developed for concrete and mortar [3], to the scale of cement paste. In the model the relevant microstructure is represented explicitly using standard continuum elastic or visco-elastic elements, while interfaces between phases as well as a sufficient number of lines in the mesh incorporate the so-called zero-thickness joint or interface elements equipped with a fracture-based constitutive model capable of consistently representing the opening and/or sliding of cracks. The model has been developed in 2D and 3D, although most application studies so far have been in 2D, because 3D calculations turn out computationally very expensive. In the present paper, this model is used to represent the micro-indentation tests with blunt spherical indenter of Portland cement pastes. As usual in any modeling attempt, this is first done in 2D to better understand capabilities and limitations at a lower, reasonable cost. Aside from the cracking model itself, this also requires to handle the contact problem between indenter and sample, which is in this case solved also using zero-thickness elements with some initial opening/sliding.

2. MICRO-MECHANICAL MODELING

A 250 µm per 250 µm image of a hydrated cement paste (175 hours age and w/c=0.30) was taken from *The Visible Cement Dataset* [4]. On this image (upper left quarter of the diagram of Fig. 1a), different components of the cement paste are represented by the various grey levels. As a first approach, for this study two different regions were manually differentiated in the image: the darker grey levels corresponding to un-hydrated clinker grains (“particles”); the lighter grey levels corresponding to voids and hydration products (high and low density CSH, portlandite, etc., “matrix”). The whole domain was meshed using linear triangles (Fig 1.b), using different material properties for particles and matrix. Zero-thickness fracture-based interface elements were inserted in between continuum elements in order to simulate the potential crack paths. This was done along all particle-matrix contacts, as well as matrix-matrix mesh lines. However, no intra-granular interfaces were considered, given the higher mechanical properties assumed for the grains themselves. The model geometry was completed with a spherical (cylindrical) indenter of radius 50 µm, a surrounding homogenized domain to avoid boundary problems, and the assumption of a vertical symmetry axis. Between the indenter and the cement paste sample, zero-thickness joint elements were also considered, with some initial opening and sliding as a first approach to model the contact problem.

The interface elements within the sample are equipped with a non-linear constitutive law capable of representing the fracture process. The law is formulated in terms of normal and shear stress tractions and the corresponding relative displacements. The initial failure surface is a hyperbola with parameters $\chi$ (tensile strength), $c$ (cohesion) and $\tan\phi$ (friction angle). After cracking opening, the evolution of these parameters is controlled by the fracture energy
spent in the developing crack, \( W^{cr} \). Other parameters required by the model are the \( G_I^{fr} \) and \( G_{IIa}^{fr} \) fracture energies. More details about this model may be found in [5] and [6].

![Figure 1: (a) 250x250 \( \mu \text{m} \) image of cement paste with water to cement ratio of 0.3 and 175 hours of hydration, taken from The visible Cement Dataset-National Institute of Standards and Technology (http://visiblecement.nist.gov). (b) Micro-scale model mesh.](image)

The calculations of indentation tests as represented in Fig. 1, were accompanied by simulations of the uniaxial tensile and compression tests, using the same micromechanical mesh and parameters as for the upper-left quadrant of the sample represented in the figure. In this way, the parameter values used or identified from indentation tests may be related to more standard parameters such as compressive or tensile strength and vice versa.

### 3. PRELIMINARY RESULTS

#### 3.1 Material parameters

All the continuum elements were considered linear elastic, with parameters estimated from values reported in the literature [7]: for the anhydrous phase (“particles”) \( E=135 \text{GPa}, \nu=0.30 \); for the hydrates’ phase (“matrix”) \( E=22 \text{GPa}, \nu=0.24 \); for the homogenized part of the mesh \( E=35 \text{GPa}, \nu=0.24 \); for the indenter \( E=10000 \text{GPa}, \nu=0.15 \). For the fracture interfaces, the parameters were set to values that would lead to reasonable behavior in the parallel simulations of standard uniaxial compression and tension tests: for the matrix-matrix interfaces \( K_n=5.0 \text{MN/m}, K_t=5.00 \text{MN/m}, \tan \phi =0.80, \chi_0=2.0 \text{MPa}, c_0=10.0 \text{MPa}, G_I^{fr}=0.10 \text{N/m}, G_{IIa}^{fr}=1.0 \text{N/m} \) and \( \sigma^{dil}=1000 \text{MPa} \), and for the matrix-particle interfaces \( K_n=5.0 \text{MN/m}, K_t=5.00 \text{MN/m}, \tan \phi =0.80, \chi_0=1.0 \text{MPa}, c_0=5.0 \text{MPa}, G_I^{fr}=0.05 \text{N/m}, G_{IIa}^{fr}=0.50 \text{N/m} \) and \( \sigma^{dil}=1000 \text{MPa} \). Finally, the interface elements along the indenter-sample contact were
considered elastic-perfectly plastic after contact is gained, with parameters $K_n=5.0 \text{MN/m}$, $K_t=0.01 \text{MN/m}$, $a = 5.0 \text{MPa}$, $\tan \phi = 10$.

3.2 Results for uniaxial tension and uniaxial compression

The results of uniaxial compression and tension simulations, using the above micromechanical parameters, are shown in Fig. 2 and Fig. 3. They lead to the following values for the overall micromechanical cement paste sample: overall elastic modulus $E_0 = 30.3 \text{GPa}$, overall initial Poisson’s ratio $\nu_0=0.246$, overall compressive strength 27.34MPa, and overall tensile strength 1.54MPa. These are all seem reasonable values for a cement paste with $w/c=0.30$ and 175h hydration time (degree of hydration approx. $\alpha \approx 0.60$).

Figure 2: Uniaxial compression test: (a) average stress/strain diagram including axial strain to the right side of horizontal axis, and lateral strain to the left side. (b) Energy dissipated in cracks.
3.3. Preliminary results for micro-indentation test

Some preliminary results obtained for this test are shown in Figures 4 and 5. In Fig.4 (left), the computed load-displacement curve is depicted together with a similar curve obtained considering the material as heterogeneous but elastic, no cracking (dashed line). The curves exhibit the expected stiffening shape as indenter-specimen contact is increased, although this effect is partially compensated by the cracking observed in the sample (solid line). As shown in Fig.4 (right), cracking reproduces a wing-shaped failure pattern with overall sideways-upper mass displacement, similar for instance to the failure patterns typical for shallow foundations. Fig. 5 depicts a detail of the displacement field near the upper surface.
4. CONCLUDING REMARKS

The results obtained show that the proposed model, which is capable of representing with a given single set of parameters the typical failure compression and tension loading, can, at the same time and with the same parameter values, also lead to reasonable representation of spherical indentation tests. This may be considered a sound basis for advanced inverse-analysis and parameter identification processes of indentation tests, finally leading to a procedure to obtain reliable and realistic mechanical and cracking parameters for cement paste at the small scale. The work presented is part of an on-going research which still needs to be improved in many aspects, such as incorporating elasto-plasticity and time-dependency in the continuum, better contact-friction representations under the indenter, considering more phases or voids in the discretized geometry, full 3D representation, etc. but in any case the results obtained so far are considered very encouraging and stimulating.

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REFERENCES


