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A COHESIVE ZONE MODEL FOR THE CHARACTERISATION OF THE INTERFACIAL TRANSITION ZONE (ITZ) BETWEEN CEMENT PASTE AND AGGREGATES

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Abstract. *Characterization of concrete behavior needs to know mechanical properties of the two phases constituting them : mortar and aggregates. Nevertheless this bi-phasic approach reaches its limits when concrete leaves the elastic domain. At that stage and according to several studies, phenomena which occur at the interface between mortar and aggregates, or in mortar between cement paste and aggregates, must be taken into account. If the occurence of an Interfacial Transition Zone (ITZ), with weak mechanical properties in regard to the two others surrounding them is well knwon, the modeling of this third phase is not settled yet. This study focus on the characterization of the adhesion at interface between cement paste and aggregates. A mortar compounded by two limestone aggregates binded by a cement paste is considered, and tensile tests are performed on a sample of this composite. Based on these experimental results, a numerical study is developed in order to see influence of interface quality in tensile strength. For thar mortar is modeled by finite elements with a cohesive zone model at the interface, substituting ITZ. With the cohesive zone model used, coupling friction and adhesion at the interface, three parameters have to be fitted : normal and tangential stiffness, and decohesion energy. A strong correlation is found between these parameters and tensile strength, but numerical results show also low values of stiffness and decohesion energy at interface. This result could be explained by a partial adhesion between mortar and cement paste in the sample.*

1 INTRODUCTION

When concrete is considered as a bi-phasic material represented at a mesoscopic scale, compounded by mortar and aggregates, the characterization of its mechanical behavior depends on elastic properties of the two phases, at less until the rupture [21, 16]. Nevertheless an acurate prediction when the elastic limit is reached is often investigated. For that, a damage variable may be introduced and the behavior is described by a volumic model as developed by Pijaudier-Cabot and Mazars [20]. These models allow to describe the post-peak behavior using inverse analysis methods [3], concrete being still represented as a bi-phasic material. In a different way, some studies consider a third phase, the Interfacial Transition Zone (ITZ) between mortar or cement paste and aggregates, as an independant material with weak mechanical properties [18]. In order to take into account this third phase, some numerical studies propose a finite element model representing physically ITZ [15, 10], inducing difficulties particularly in the mesh generation because of the very thin thickness of ITZ in regard to dimensions of other phases [4]. In their experimental and numerical studies, Ke et al. [12, 13] have overcome these difficulties with the development of a micromechanical model, especially for lightweight concrete, in order to predict failure. Other works consider a mechanical damage induced by the quality of the matrix-aggregates interface [14]. In the present study we focus on the caracterization of the mechanical link between cement paste and aggregates.

A non perfect adhesion between two phases, may be modeled by introduction of Cohesive Zone Models (CZM) at the interface. These models provide good description of mechanical behavior, also out of elastic domain [6]. Among various studies using CZM in their numerical models, based on finite elements modelling [17, 7, 23] or with discrete elements [1], the one used in this paper, couples adhesion, friction and unilateral contact [22, 24]. Here, cohesive forces directed at interface are both in tangential and normal directions [2]. Cohesion at interface is represented by a damage parameter β, providing the intensity of adhesion.

The work presented here, deals with a characterization of interface quality, between cement paste and limestone aggregate. For that, the cohesive zone model quoted previously is calibrated on mechanical tests performed on a composite compounded by two cubic samples of limestone linked by a thin thickness of cement paste. For that a three-dimensionnal finite elements model of the composite is carried out using the software LMGC90 [5]. Parameters of CZM law fitted will describe the mechanical properties and the adhesion quality at the interface between cement paste aggregates.

2 MATERIALS AND METHODS

2.1 Experimental sample of concrete

All experimental results come from works of PhD thesis of Mouad Jebli, from University of Montpellier, France. Composite of mortar is realized with two cubic blocks of limestone binded by a thin cement paste, as represented in the Figure 1. Elastic properties of these two materials are obtained by uniaxial compression tests and are summarized in the Table 1.

Material	Young's modulus (GPa)	Poisson ratio
Limestone	60	0.3
Cement paste	12.5	0.3

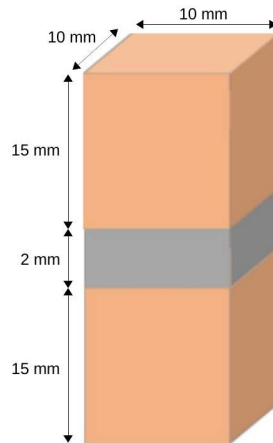Table 1: Elastic properties of aggregates and cement paste

Figure 1: Sample of concrete compounded by two blocks of limestone ($10 \times 15 \times 10$ mm) binded by a cement paste ($10 \times 2 \times 10$ mm)

Mechanical tensile tests are carried out on the sample. A velocity of 0.01 mm/s is imposed through a tensile test device, as shown by the Figure 2. Sample is loaded until rupture. The onset of cracking and rupture of the sample is recorded with use of a high-speed digital camera. For the calibration of the cohesive zone model, results on 28 days mortar composites have been taken into account.

Figure 2: Tensile test on the concrete sample

Results of uniaxial tensile test are shown on Figure 3. This curve will be used on the following to choose parameters of CZM at the interface.

2.2   Cohesive Zone Model

Mathematical developments of the model chosen here, using thermodynamic considerations, are detailed on several works [2, 22]. We will limit in this part to present parameters of the cohesive law, and its main constitutive equations. This model considers a non-penetration between two bodies in contact, here cement paste and aggregates. These two materials are meshed by finite elements. The unilateral contact is coupled with friction, coming from Coulomb law be-
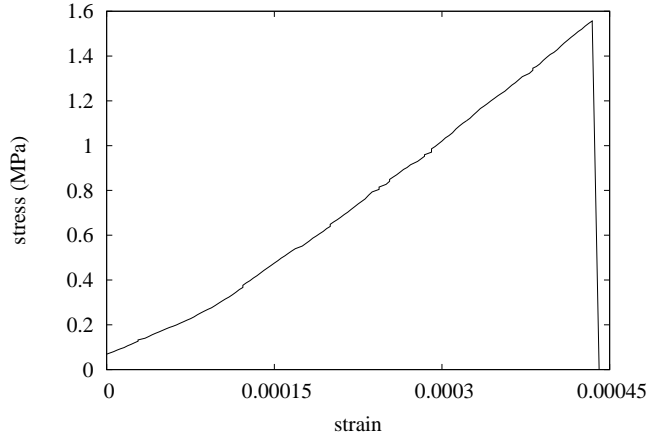
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Figure 3: Stress (in MPa) vs strain for tensile test on the concrete composite

tween the two materials, and adhesion governing by a state variable which describes the contact state. This variable β, introduced by Fremond [9], giving the intensity of adhesion between the two bodies in contact, is defined with a damage parameter D included between 0 (no damage) and 1 (rupture) such as :

$$\beta = 1 - D \tag{1}$$

Thus adhesion linked to damage between aggregate and cement paste is :

- $\beta = 1$ total adhesion

- $0 < \beta < 1$ partial adhesion

- $\beta = 0$ no adhesion

The thermodynamic description, based on standard material generalized theory [11], needs to define state variables associated to thermodynamical forces. For that one considers the reversible forces R_N and R_T associated to the dispalcements u_N and u_T. Indexes N and T indicate a decomposition into normal and tengential part on the contact surface. Thus, R_N and R_T are considered as normal and tengential contact forces and the displacement is written :

$$[u] = [u_N] \, . n + [u_T] \quad \text{with} \quad [u_N] = [u] \, . n \tag{2}$$

In a same way, the decomposition of contact forces gives :

$$R = R_N . n + R_T \quad \text{with} \quad R_N = R . n \tag{3}$$

In this problem the state variables are β, u_N and u_T, and we introduce a free energy potential defined such as :

$$\psi(u_N, u_T, \beta) = \frac{C_N}{2} u_N^2 \beta^2 + \frac{C_T}{2} u_T^2 \beta^2 - wb \tag{4}$$

4

with C_N and C_T the normal and tengential stiffness, w the Dupre's energy and b the adhesion viscosity coefficient. As explained in works of Raous et al. [22], the main constitutive laws of the contact at the interface come from the subdifferentiation of the free energy potential, and a potential of dissipation, with respect to the state variables u_N, u_T and β. As consequence we can define the unilateral contact with adhesion :

$$
\begin{aligned}
R_N - C_N \left[u_N\right] \beta^2 &\geq 0 \\
\left[u_N\right] &\geq 0 \\
\left(R_N - C_N \left[u_N\right] \beta^2\right) \left[u_N\right] &= 0
\end{aligned}
\tag{5}
$$

Introducing a fricton coefficient of Coulomb μ, the friction with adhesion is defined by the following equations :

$$
\begin{aligned}
||R_T - C_T \left[u_T\right] \beta^2|| &\geq \mu |R_N - C_N \left[u_N\right] \beta^2| \\
||R_T - C_T \left[u_T\right] \beta^2|| &< \mu |R_N - C_N \left[u_N\right] \beta^2| \Rightarrow [\dot{u_T}] = 0 \\
||R_T - C_T \left[u_T\right] \beta^2|| &= \mu |R_N - C_N \left[u_N\right] \beta^2| \Rightarrow \exists \lambda > 0, [\dot{u_T}] = \lambda(R_T - C_T \left[u_T\right] \beta^2)
\end{aligned}
\tag{6}
$$

Finally, shape of the cohesive law presented is shown by the curve of the Figure 4 giving the normal reaction with respect to normal displacement. Force-peak represents the limit of adhesion. Indeed at that stage damage occurs at interface, and energy of adhesion, considered as the area under the cruve decreases.
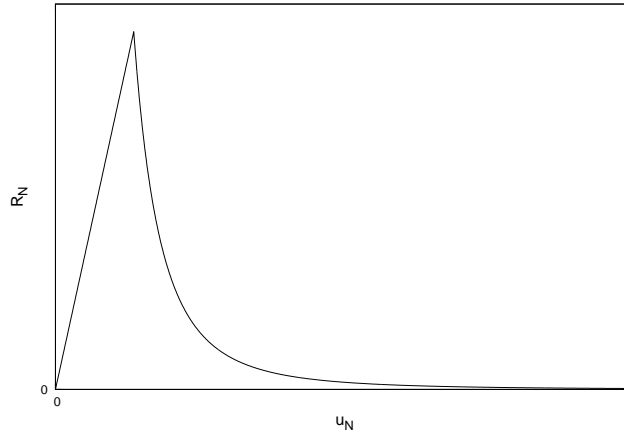

Figure 4: Shape of the cohesive law

2.3 Numerical computation

All the numerical computations have been proceeded with the open software LMGC90 [5], developed at the University of Montpellier, France, in which the cohesive zone model presented in past section is implemented. A tree-dimensional finite element model of the composite sample has been carried out. A symmetrical geometry has been chosen, as shown by Figure 5, in order to reduce computation time, thus conditions of symmetry will be respected. Geometry is

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meshed with hexaedron finite elements H8, and the time step is taken constant and equals to 1×10^{-4} s. A theta-method is chosen for time intregation with $\theta = 0.55$. Boundary conditions are applied on the lower and upper faces, with a velocity $v_y = 0.01$ mm/s for the tensile load on the upper, and vertical displacements blocked on the lower due to symmetry.
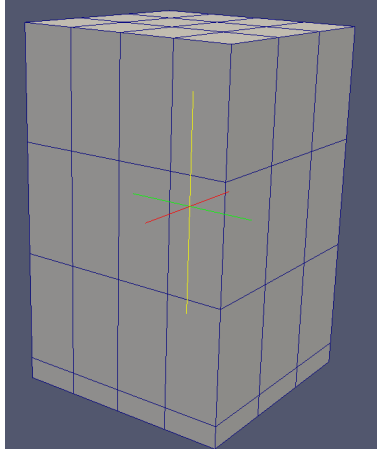

Figure 5: Meshing of a half composite sample by hexaedron finite elements

Application of the cohesive zone between cement paste and aggregate, is based on contact nodes placed in the contact surface both on cement paste and aggregates. At each time step a detection is realised and rupture occurs when contact is lost between the two bodies. To calibrate cohesive law, several parameters have to be setted : normal and tangential stiffness C_N and C_T, friction coefficient μ, adhesion energy w and adhesion viscosity b. In this model we consider any viscosity at the interface, thus $b = 0$. Friction coefficient is determined by experimental study, and $\mu = 0.4$. We assume that adhesion energy, is defined by the experimental curve stress-strain (Figure 3), and calculated as the aera under the curve, until the rupture. Hence :

$$w = \frac{1}{2}(1.6 \times 10^6 \times 0.015 \times 10^{-3}) = 12 \, \text{J/m}^2 \tag{7}$$

Hence, adhesion energy calculated here is only the one for the elastic part until rupture, thus according to the Figure 4 presented in the past section we assume that the value corresponding in the cohesive law is near the double, $24 \, \text{J/m}^2$. We will see in the following if this assumption gives results expected.

Finally, only C_N and C_T have to be fitted with the experimental results. We assume that $C_N = C_T$, hence their value will be calibrated with several numerical tensile test on the composite sample.

3 RESULTS

Numerical computation is performed until the peak-stress, and compared with the experimental stress-strain curve, the objective being to tend to this curve. On the finite element model, we observe that rupture is represented by a decohesion between the two bodies, as shown by the Figure 6.

As explained previously, in this study two parameters have to be fitted : C_N, C_T. It appears that in our case, C_N and C_T give the slope of the linear par and the w sets the position of
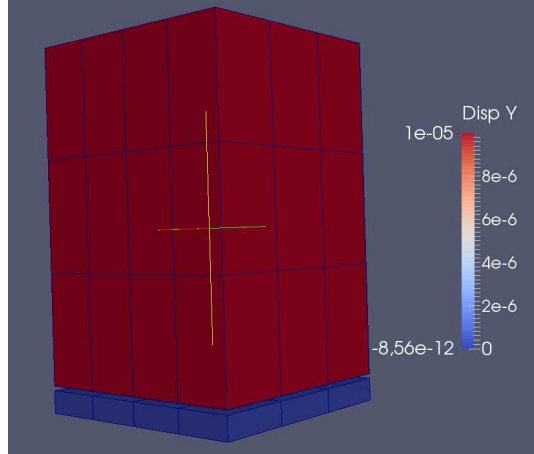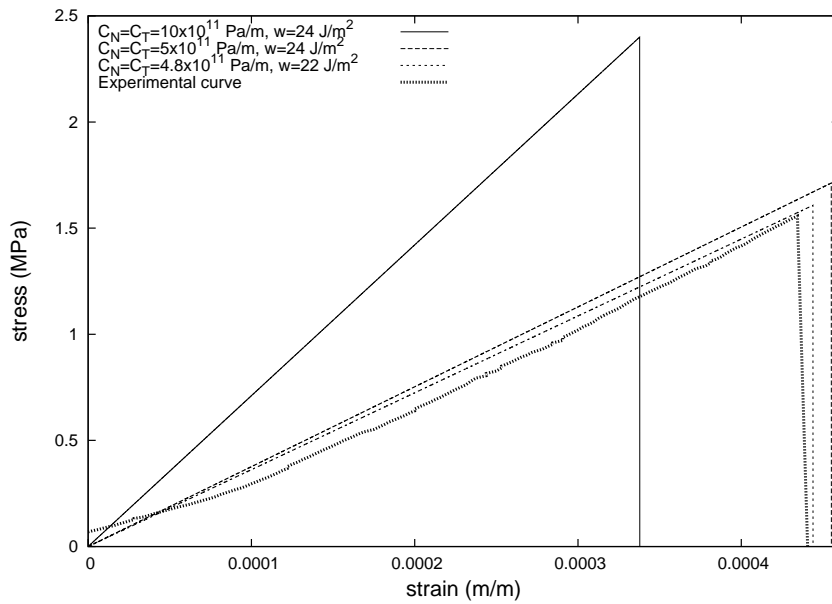
Figure 6: Displacement of the two materials after rupture

peak stress along the slope. Influence on these three parameters on the mechanical response are represented of the Figure 7. Value of decohesion energy estimated previously, has to be slightly reduced to bring numerical peak stress closer to the experimental one.

Figure 7: Influence of parameters C_N, C_T and w on the mechanical response

Thus, we can observe on Figure 7 that paramaters of cohesive zone model which allow to tend to experimental curve are $C_N = C_T = 4.8 \times 10^{11}\,\mathrm{Pa/m}$ and $w = 22\,\mathrm{J/m^2}$.

4   DISCUSSION

We can first notice a strong correlation between mechanical parameters defined at the interface between cement paste and aggregates, and both strain and tensile strength. Moreover numerical results show that with this cohesive zone model, it is possible to tend to experimental results. We can observe that value of decohesion calculated experimentaly, gives a good estima-

tion of the peak stress. The slightly decrease is explained by the interface considered as perfect in the numerical sample which is not the case in the experimental one. As consequence with w fixed by the experiment, only 2 parameters have to be fitted.

Since decohesion occurs only in the ITZ, the latter is substituted by cohesive zones. Thus parameters fitted can be considered as characteristics of the ITZ. A comparison with other studies realised with the same cohesive law, give values of interfacial stiffness higher than the one obtained here. Indeed works of Perales et al. [19], have shown that $C_N = C_T = 2 \times 10^{18}$ Pa/m when studies of Fouchal et al. [8] found 1.5×10^{17} Pa/m. These values depend on material modeled, hydrided Zircaloy for the first and interface between bricks and mortar for the second. In the same way, our values of decohesion energy are also weak, particularly comparing to adhesion between bricks and mortar $(0.9 \, \text{J/mm}^2)$. Two ways may be investigated to explain these low values of interface parameters : parameters identified with numerical computation are not representatives of the real interface properties, or an initial damage occurs at the interface, due to the composite sample fabrication. If the first hypothesis requires other experimental investigations, in particular on a mini-structure of mortar, let us focus on the second through an analysis of Young modulus.

Experimental Young modulus of the composite sample, could be calculated as being the slope of the curve of the Figure 3. Indeed, assuming that until tensile strength, in the linear part, the sample has an elastic behavior, Young modulus is obtained using the Hooke law for an uniaxial tensile test :

$$E_{sample} = \frac{\sigma}{\varepsilon} \tag{8}$$

with σ the stress and ε the strain. Here, according to the Figure 3, $E_{sample} = 3.43$ GPa. This value has to be compared with the real Young modulus of the sample, which could be calculated through a serial stiffness. Indeed if we consider that the sample is compounded by three serial elastic bodies, the equivalent stiffness is defined by :

$$k_{sample} = \frac{1}{\frac{2}{k_{agg}} + \frac{1}{k_p}} \tag{9}$$

where k_{agg} and k_p are aggregate and paste stiffness defined such as :

$$k_{agg,p} = \frac{S_{agg,p} \times E_{agg,p}}{L_{agg,p}} \tag{10}$$

with $S_{agg} = S_p = 100 \, \text{mm}^2$ the section of aggregate and cement paste, $L_{agg} = 15 \, \text{mm}$ the length of each aggregate and $L_p = 2 \, \text{mm}$ the length of the paste. Thus using these values, composite stiffness is $k_{sample} = 151515 \, \text{N/mm}$ leading to the theoretical equivalent Young modulus of the sample :

$$E_{th} = \frac{32 \times 151515}{100} = 48.5 \, \text{GPa} \tag{11}$$

A noticeable difference is observed between theoretical Young modulus and the one obtained experimentally. This result may be explained by a damage at the interface, due to the interface

quality between aggregate and cement paste, which lead to a fall on the equivalent Young modulus. According to the definition of the damage variable given by Mazars et al. [20], theoretical and experimental Young modulus are binded by the relationship :

$$E_{sample} = (1 - D)E_{th} \qquad (12)$$

where the damage variable D is different to zero, inducing an intensity of adhesion β less than 1 at the begining of the computation, as explained by equation (2.2). This observation could indicate a partial adhesion between aggregate and cement paste and explain low values of stiffness and decohesion energy at the interface. Thus the strong correlation between stiffness and adhesion energy at interface, and mechanical behavior of the composite, leads to confirm that tensile rupture is in this case governing by the adhesion quality.

5   CONCLUSION

Cohesive zone model applied to the numerical computation studied here, allows to calibrate decohesion between cement paste and limestone aggregate, using experimental tensile test on a composite sample compounded by both materials. It is possible to reach experimental stress-strain curve, with values of stiffness at the interface and decohesion energy according to literature. Moreover Young modulus obtained by experimental works and numerical computation, calculating the slope of the stress strain curve, is very small against the theoretical one. Other experimental studies have to be performed to confirm the existence of initial damage at the interface.

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