

# From discontinuous to macroscopic modeling of mode I cracking behavior in cement-based composites

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**ABSTRACT:** this paper puts forward the basic ideas of an original approach for modeling the cracking behavior of cement-based composites: arising from results of numerical simulations representing the – discrete and probabilistic – cracking behavior of concrete in tension, the mechanical uniaxial pre-peak and post-peak responses are analyzed in statistical terms. Information thus obtained is implemented in a simplified macroscopic modeling of the material mechanical behavior.

## 1 INTRODUCTION

Although models are more and more sophisticated and relatively appropriate to represent the macroscopic mechanical behavior of concrete structures, they are not usually fully pertinent for providing information on the characteristics of the cracks: opening, orientation and spatial distribution. The knowledge of these characteristics is of great importance if, for example, the durability of the structure is considered. It is now well known that the properties of transfer of the material, gas or liquid permeabilities or diffusion coefficients, are impacted by cracks: openings or the density of cracks are essential factors that have to be taken into account in the modeling of physical transfers. This can be considered as an important condition for estimating the lifespan of the structure, through an accurate prediction of its durability. In terms of modeling, difficulties appear in the link which must be set up between the local description of the mechanisms and the global response of the structure, essentially when their combination is challenged through a robust and reliable modeling.

## 2 MODELLING CRACKING PROCESSES AT DIFFERENT SCALES

The starting point of this study is the execution of a broad numerical experimentation aimed at studying the tensile behavior of a large range of concretes. These numerical simulations are based on the discrete and probabilistic approach developed by Rossi and co-workers. (Rossi & Richer 1987, Rossi & Wu

1992, Rossi et al. 1996, Rossi & Ulm 1997). This model is designed to describe the onset and the propagation of cracks and also to take into account volume effects. The model is based on the hypothesis considering that the mechanical properties of the concrete, like the young modulus and the tensile strength, are related to the major heterogeneity, represented by the coarsest grain, and the initial defects influencing the (mechanical) quality of the cement paste. These observations are detailed in (Rossi et al. 1994), where authors conclude that the young modulus and tensile strength are statistical variables following normal (Gaussian) laws and depending on only two parameters: the first one is the ratio between the volume of the specimen and the volume of the coarsest grain ( $V_s/V_g$ ) and the second is the compressive strength of the concrete ( $f_c$ ). The characteristics of the statistical distributions, mean values and standard deviations, are then given by empirical formulas deriving from the experimental observations. The reader will find their mathematical expressions in the previous references, for example. One can note that these formulas can be rigorously considered as valid in a limited domain corresponding to the one which was experimentally explored, i.e. for Equation 1 and Equation 2:

$$\begin{cases} 10 \leq \phi_d \leq 25 \text{ mm} \\ 35 \text{ MPa} \leq f_c \leq 130 \text{ MPa} \end{cases} \quad (1)$$

where  $\phi_d$  = diameter of the coarsest grain. And:

$$10 \leq V_s/V_g \leq 7000 \quad (2)$$

One can also notice that this domain of validity can cover large ranges of concrete formulations and of laboratory specimen geometries.

The numerical implementation of this model takes place in the general framework of the finite-element method. The uncracked concrete is modeled using massive triangular elements while contact elements, which interface them, represent cracks. Then the model accounts for cracks as geometrical discontinuities. The stochastic process is introduced at the local scale by considering that cracks are open in the material with different energy dissipations due to the heterogeneity of the material. Considering that the local behavior of concrete can be elastic-perfectly brittle, the random space distribution of local fracture energies can be replaced by a random space distribution of local tensile strengths. Since the mechanical properties are considered as random variables, they are distributed on the mesh according to distribution characteristics following the empirical formulas.

The model is actually implemented in 2D in the expert version of the finite element code CESAR-LCPC (Humbert 1989).

The underlying, and basic, idea of the model is then to consider a finite element volume like a material volume and to assume that physical mechanisms influencing the cracking processes remain the same whatever the scale of observation. Then the volume of the specimen ( $V_s$ ), in empirical formulas cited above, is replaced by the volume of the element ( $V_e$ ), and the young modulus and the tensile strength of the finite (material) element are deduced from these formulas. According to the local and probabilistic character of the approach, the volume of the element must be sufficiently small in comparison to the volume of the meshed structure or in comparison to the zone size where stress gradients can develop. This can lead to very small ratios  $V_e/V_g$  being out of the initial domain of validity. In fact, Tailhan and co-workers (Tailhan 2006) have shown that the evolutions of the mean values and the standard deviations given by the empirical formulas with respect to the compressive strength become false and physically inadmissible for ratios  $V_s/V_g$  smaller than one. Then, they have proposed to perform an inverse analysis to determine the extrapolation of the empirical formulas to the small ratios  $V_e/V_g$  domain. Note that a similar work was performed in (Fairbairn et al. 2000), but for larger ratios  $V_s/V_g$ .

The principles of this inverse analysis are summarized in the diagram (Figure 1). For a given concrete type and a given volume of specimen (1), the mean value and the standard deviation (2) of the distributions of mechanical properties (young modulus and tensile strength) at the level of the finite elements are researched in order to obtain mean values and standard deviations (3) computed on the global responses of the specimen, in accordance with the prediction given by empirical formulas (4) in their validity domain.

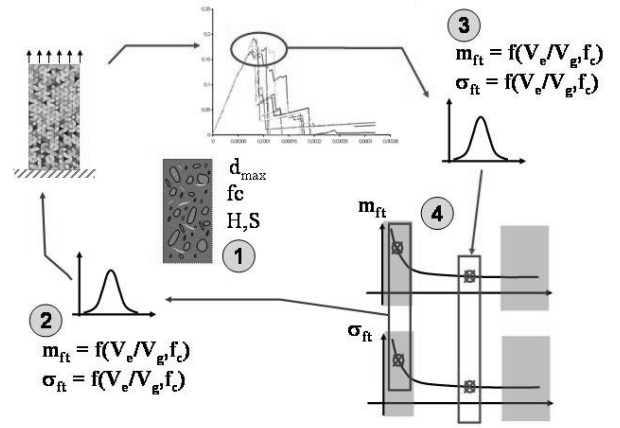


Figure 1. Principle of the inverse analysis

Many simulations are performed with different geometries of specimens, different diameters of coarsest grain and different values of compressive strength. 15 computations are performed for each configuration, so that a statistical analysis of the results can be done. Simulations are also performed in 2D plane stress. For a sake of simplicity, our attention is only focused on the tensile strength, which is considered to be the only random variable. The elastic properties of the materials are maintained constant and are deduced from classical estimation formulas:

$$E = 11000\sqrt[3]{f_c} \quad \text{and} \quad \nu = 0.2 \quad (3)$$

Meshes, which are used in this inverse analysis, are shown in Figure 2. For all computations, the thinness of the meshes remains the same: ratios between the sizes of the elements and the sizes of the meshes are kept constant and equal to  $1.74 \cdot 10^{-3}$ .

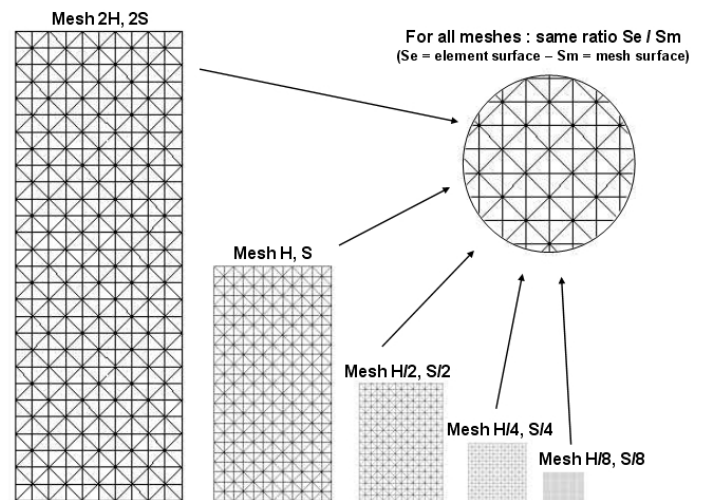


Figure 2. Meshes used in the inverse analysis. ( $H=0.276$  m and  $S = 1.910 \cdot 10^{-2}$  m<sup>2</sup>)

The  $V_e/V_g$  ratios, which are examined, are equal to 10, 1 and 0.1. The values for  $f_c$  used in the simulations are: 40 MPa, 80 MPa, and 100 MPa.

All the results of this study are reported in (Tailhan 2006). They mainly show the feasibility of the method.

Another complementary study is currently under development, in which an optimization procedure is used to automatically determine the distribution characteristics at the element scale. This procedure is based on the so-called Nelder-Mead algorithm, itself based on the simplex method (Mathews 2004). All the details of the study will be soon published.

However, we report here some of the major results of the initial study. For example, Table 1 shows results obtained for one type of concrete ( $f_c = 40$  MPa) and different ratios  $V_e/V_g$  (0.1, 1, 10). They clearly show the auto coherence of the model: if one imposes, at the level of the element, the mean values and standard deviations indicated in this table, one obtains, at the level of the global mesh representing the specimen, mean values and standard deviations similar to those predicted by empirical formulas (Rossi 1994).

Geometries	H/4,S/4	H/4,S/4	H,S
$\phi_d$ (m)	0.022	0.010	0.012
$V_e/V_g$	0.1	1	10
$V_s/V_g$	58.9	574.2	5809.3
Mean value and standard deviation imposed at the level of the element:			
m(ft)	6.7	5.6	4.3
$\sigma$ (ft)	3.0	2.7	1.1
Mean value and standard deviation obtained for the concerned specimen:			
m(ft)	3.4	2.8	2.5
$\sigma$ (ft)	0.7	0.25	0.2
Mean value and standard deviation given by the empirical formulas:			
m(ft)	3.8	2.9	2.2
$\sigma$ (ft)	0.6	0.3	0.14

Table 1. Auto coherence of the model after the inverse analysis. Results obtained for  $f_c = 40$  MPa.

Figure 3 also shows the availability of the model to represent scale effects: results also correspond to one type of concrete ( $f_c = 40$  MPa) and different geometries. One can observe that the peaks of all the curves are different, although the concrete is the same. The tensile strength increases when the volume of the material decreases, which is in accordance with the model hypotheses. A similar remark can be made on the post-peak behavior which appears to be less brittle for small volumes of material. Taking into account the heterogeneity of the material, the post-peak behavior can be related to local

stress concentration. For small volumes of material, the zones, where stresses are concentrated, are of a size relatively close to the one of the specimen. Local failure can occur if stresses reach inadmissible values. But, these values are related to inner defects of the material. The more important the size of the concentrated stress zone is, the greater is the number of inner defects taking place in the cracking process. This can also explain the more diffuse crack pattern in the case of small volumes of material. One can also note that coarsest grains are playing an important role in limiting the crack propagation, or by bridging the crack lips leading to an increase of dissipated energy by the cracking process.

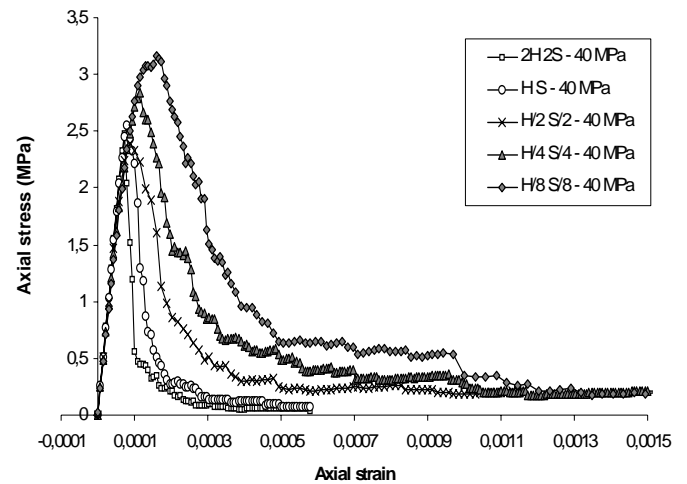


Figure 3. Illustration of the size effects on the axial tensile behaviour of concrete (in the case of  $f_c = 40$  MPa) for different sizes of specimens. Each curve represents the mean curve of 15 simulations, (from Tailhan 2006).

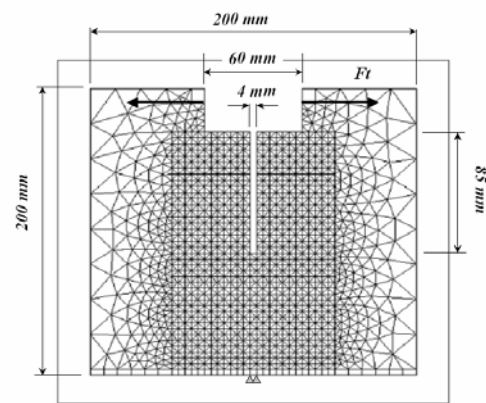


Figure 4. Mesh used for the simulation of the wedge splitting test performed in Denarié 2000.

Another interesting result recently obtained using this model is reported below. The wedge splitting test performed in (Denarié 2000) is simulated here. Input data of the model are relatively simple: the young modulus, the compressive strength and the

diameter of the coarsest grain. The diameter is given by the formulation of the concrete; the young modulus and the compressive strength are experimentally determined. Therefore, these parameters are:  $E = 25200\text{Mpa}$ ,  $f_c = 50\text{Mpa}$ ,  $\phi_d = 8\text{mm}$ .

Figure 4 shows the mesh which is used. And Figure 5 shows the comparison between experimental and numerical results, in terms of mean curves. And finally, figure 6 shows an example of the crack path obtained at the end of the simulation.

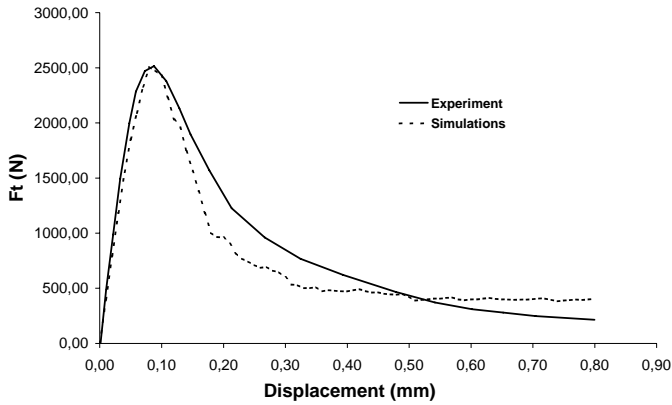


Figure 5. Comparison between experimental and numerical results for the wedge splitting test.

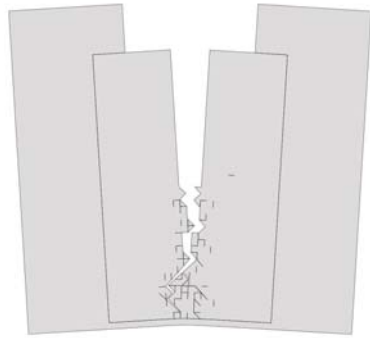


Figure 6. Crack path at the end of the simulation.

All these results clearly illustrate the availability of the model to represent cracking processes and volume effects in cementitious composites.

The strong points of the model are then, firstly, the low number of input data which can be easily determined by very classical experimental tests, and secondly, the fact that the model can give local information on cracks (crack mouth opening, cracks distribution ...)

Its weak point is essentially the fact that this model is not really well suited for the simulation of big structure behavior (impressive number of elements, high computation costs).

### 3 A SIMPLIFIED MACROSCOPIC MODELING OF CRACKING PROCESSES AND VOLUME EFFECTS

One way to avoid these problems could be to combine the robustness and efficiency of a macroscopic modeling of the behavior of concrete structures with the strong points of the discrete and probabilistic model, described in the preceding section.

One way to achieve this task is to perform a large numerical experimentation campaign and analyze its results. This point is actually being examined in pure tension.

On the bases of results such as those shown in Figure 3, pre-peak and post-peak responses are examined in statistical terms. Mean values and standard deviations of characteristics quantities describing pre- and post-peak behaviors are identified. These quantities can be for example the tensile strength and something like a “density of inelastic deformation energy”, represented by the area under the curve stress-inelastic strain.

Therefore, a series of  $n$  computations per configuration (geometry and type of concrete) can be performed. They use the previous probabilistic and discrete cracking model and process results of each of them as indicated above. Figure 7 shows the response of the simulation in terms of stress – strain mean curve for the HS specimen (see Figure 3) and for  $f_c = 30\text{MPa}$  and  $V_e/V_g = 10$ . Each point of this curve represents the mean value of points of 30 different simulations.

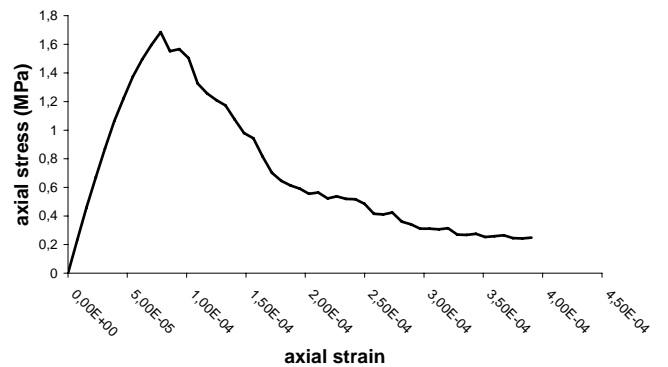


Figure 7. Axial stress vs. Axial strain curve for the HS specimen (see Figure 3) and corresponding to  $f_c = 30\text{MPa}$  and  $V_e/V_g = 10$ .

The post-peak behaviors of the 30 simulations are considered to begin at the maximum stress of each simulated stress – strain curve. The “inelastic strain” is then computed as the difference between the total strain and the elastic strain, i.e.:

$$\varepsilon_{in} = \varepsilon - \varepsilon_{el} = \varepsilon - \frac{\sigma}{E} \quad (4)$$

For each simulation, a curve stress – inelastic strain is obtained, and the area under this curve is computed:

$$W = \int_0^{\varepsilon_{in\lim}} \sigma d\varepsilon_{in} \quad (5)$$

where  $W$  = area and  $\varepsilon_{in\lim}$  = limit inelastic strain. This limit corresponds to a certain value of inelastic strain at which one can consider the total failure of the specimen.

Therefore,  $W$  can be considered as a random variable and a mean value and a standard deviation can be computed for  $W$ . The evolutions of this mean value and this standard deviation are plotted versus the inelastic strain on Figure 8 and Figure 9 (for one type of concrete:  $f_c = 30$  MPa and  $\phi_d = 0.015$ )

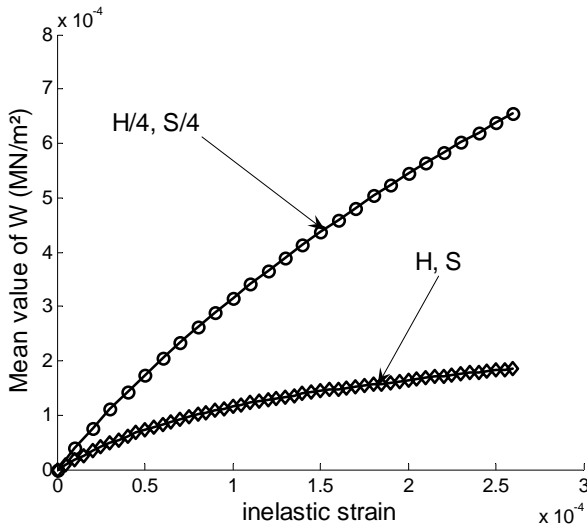


Figure 8. Evolution of the mean value of  $W$  vs. inelastic strain.

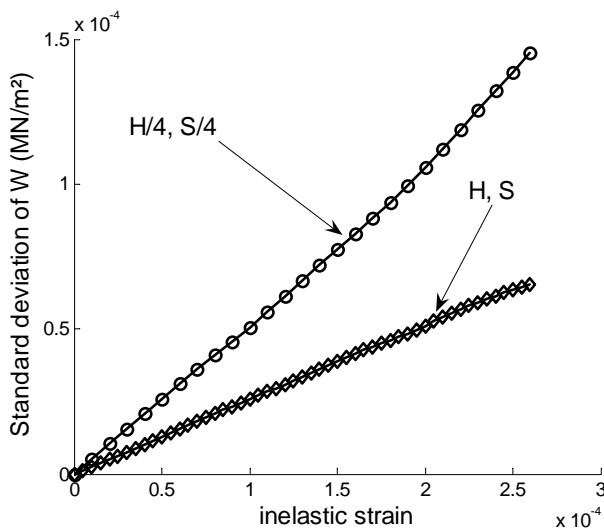


Figure 9. Evolution of the standard deviation of  $W$  vs. inelastic strain

One can observe on figure 9 the increase of the dispersion when the strain also increases. This can be interpreted by the fact that when the crack propagates through the specimen, the resisting section de-

creases, then the ratio  $V/V_g$  also decreases and therefore, according to the hypotheses of the model, the dispersion consequently increases.

The macroscopic model which is used in this study is relatively simple. It is based on the classical framework of the elasto-plasticity. The concrete, submitted to a pure tension, is assumed to follow an elasto-plastic behavior. A very simple criterion is adopted: the plastic strain begins to occur when the maximal principal stress is reached. Therefore, the plastic strain evolves as long as a limit value is reached. This limit value corresponds to the value of  $W$  at which the concrete is considered as being totally failed. As shown in Figure 8 and Figure 9, the mean value and the standard deviation of  $W$  depend on the size of the specimen, then, they also depend, for one type of concrete, on the ratio  $V_g/V_g$ .

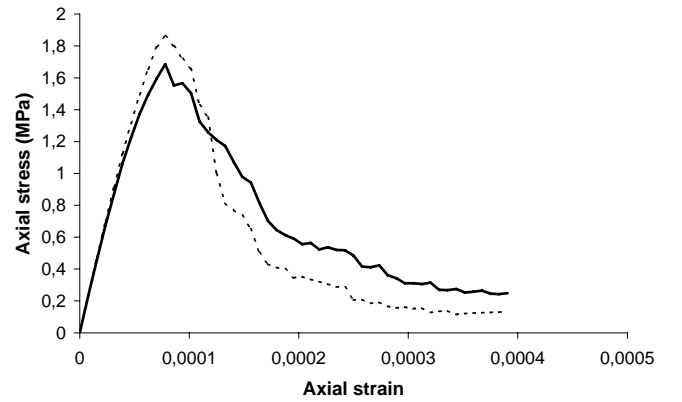


Figure 10. Comparison between both approaches: macroscopic (dashed line) and discrete (solid line) for the H,S specimen and a concrete formulation given by  $f_c = 30$  MPa and  $\phi_d = 0.015$

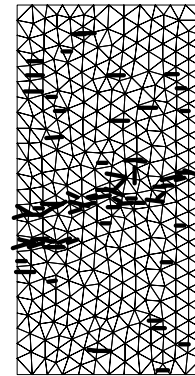


Figure 11. Example of crack pattern at the end of a simulation for the H,S specimen and a concrete formulation given by  $f_c = 30$  MPa and  $\phi_d = 0.015$

Considering, again, a finite element volume like a material volume and assuming that physical mechanisms influencing the cracking processes remain the same whatever the scale of observation, the tensile strength and the density  $W$  are randomly distributed on the elements. And again, a series of 10 simulations is performed. Results in terms of mean curve

are compared to results obtained using the discrete approach (Figure 10). And an example of crack pattern is also shown on Figure 11.

#### 4 CONCLUSION

On the basis of a probabilistic and discrete modeling, the cracking processes occurring in concrete specimens under tension are analyzed. They clearly show that the behavior of concrete is highly influenced by its inner heterogeneity and the initial defects in the material, exhibiting therefore, strong volume effects. This approach is based on the main hypothesis that the physical mechanisms taken into account in the model at the scale of the material are representative of the one at the scale of the specimen. This kind of approach makes it possible to perform a real numerical experimentation of the axial behavior of the material. Pre- and post-peak behaviors are then analyzed in statistical terms. Mean values and standard deviations of the tensile strength (and also those of the young modulus) are related to the compressive strength and to the ratio volume of material to volume of the coarsest grain. The analysis of the post-peak behavior can lead to the same remark concerning the mean evolution and the dispersion which were noted.

On that bases, principles of a simplified macroscopic modeling of the uniaxial behavior of concrete are given. This kind of approach will deal mainly, in the long term, with the structural analysis.

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