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Université Grenoble Alpes

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E. Roubin[1]

[1] *LMT–Cachan, Ecole Normale Supérieure de Cachan, Université Paris VI, CNRS, UniverSud Paris, 61 avenue du Président Wilson, 94235 Cachan Cedex, FRANCE*
emmanuel.roubin@lmt.ens-cachan.fr

Prix Jeunes Chercheurs « René Houpert »

RÉSUMÉ. *À des échelles d'observation fines (inférieures à l'échelle centimétrique) les matériaux à matrice cimentaire ne peuvent plus être considérés comme des milieux homogènes. Ils sont, dans le cadre de cette étude, considérés comme bi-phasiques, les granulats étant inclus dans une matrice cimentaire. Deux problématiques majeures qu'entraine cette thématique de modélisation sont abordées. D'un coté la modélisation morphologique et d'un autre, la modélisation mécanique prenant en compte le caractère hétérogène et quasi-fragile du matériau. Le résultat principal de l'étude montre que la simple modélisation de la morphologie permet, avec des modèles mécaniques simples, de retrouver des comportements macroscopiques complexes. Une application est faite montrant l'impact des incompatibilitées de déplacement entre la pâte de ciment et les granulats du au retrait de séchage sur la dissymétrie du comportement en traction/compression du béton.*

ABSTRACT. *A 3D meso-scale model for failure of heterogeneous quasi-brittle materials is presented. At such scale, concrete can be represented as an heterogeneous material with two phases, where inclusions (aggregates) are included within the matrix (mortar). Both morphological quasi brittle failure mechanism modelling are expressed here. Finally, impact of drying shrinkage incompatibilities between aggregates and cement paste on asymmetrical response in tension/compression tests is shown.*

MOTS-CLÉS : *Matériaux hétérogènes, modélisation morphologique, comportement quasi-fragile*

KEYWORDS: *Heterogeneous materials, Morphological modelling, quasi-brittle mechanism*

1. Introduction

In view of the growing complexity of macroscopic models for heterogeneous materials, such as concrete or more generally cement-based ones, the question of scale observation becomes relevant. On the one hand, it clearly appears that most of the macroscopic behaviours of such materials (creep, shrinkage, cracking. . .) take their origin at smaller scales (mesoscopic, microscopic. . .). Hence, predictive and accurate numerical simulation of long-term behaviour related to concrete structures durability shall account for these scales. On the other hand, usage of very fine imaging procedures, mostly inspired from the medical field, with concrete-like materials has increased dramatically over the last few years. Chief among them is the X-ray tomography [ROU 10] which offers a nondestructive way to get very precise data, dealing with both morphological and mechanical aspects. Numerical simulations shall be able to use this huge volume of data for both parameter identification and validation of numerical models.

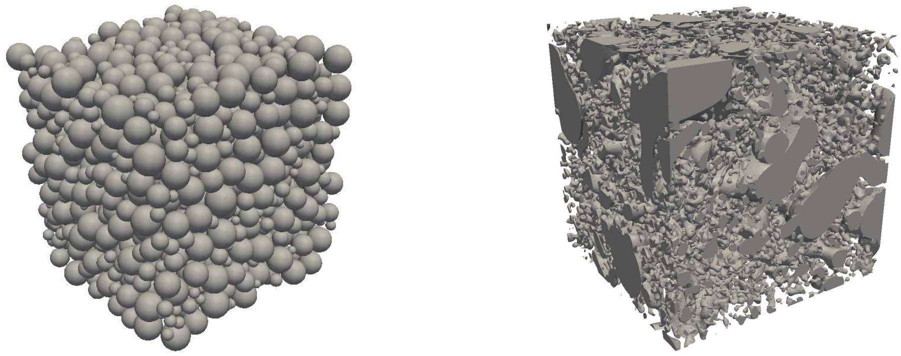
The framework presented here is to be seen in this context, and especially within a sequenced multiscale way (as opposed to integrated ones) where the macroscopic behaviour comes from a mesoscopic description of the material. In other words, we consider the macrosocopic mechanical behaviour of such material as a *complex system*. It is assumed that the final result cannot be predicted directly. A way of dealing with such systems is to set several basic evolution rules and simulate the system in order to obtain the structured final result. In our case, this result is the macroscopic behaviour and the basic rules are defined by the mesoscale description. This point of view can also be seen as *virtual testing* procedure.

At fine scale, concrete must be represented as a heterogenous materials. Therefore, two kinds of basic rules need to be established in such framework. The first kind is a purely geometrical and topological matter with the aim of explicitly representing, as faithfully as possible, the morphology of material heterogeneities. The random aspect of this representation links our virtual testing framework with Monte Carlo experiments. The second kind of basic rules is purely mechanical and defines the local behaviours of each phases of the material and their interfaces. A quasi-brittle failure mechanism is wanted, adding a strongly non-linear aspect to the system. Both kind of representation of the meso-scale are complex (random heterogeneities and non-linear behaviour) yet one have to keep in mind that those two aspects are completely independant.

The global spirit of the whole framework is to consider that with a representative morphological description, the mechanical behaviour of each phase can be kept as simple as possible and still lead to complex macroscopic behaviour. For example, it is shown in this work that with a simple brittle tension failure mechanism at the mesoscale, macroscopic compression failure can be simulated.

2. Explicit representation of the meso-scale heterogeneities

In this work, the mesoscopic scale characteristics are explicitly defined. Therefore a special effort had to be made concerning the morphological representation of heterogeneities. Two characteristics shall be considered concerning this modelling. First, the geometry and topology has to fit as close as possible to reality (volume fraction, area fraction, number of aggregates, size repartition...) and secondly, the random aspect of aggregates repartition within the matrix has to be explicitly represented. Two different methods of heterogeneity morphological representation are quickly overviewed. The first one represents aggregates with non-intersecting spheres of various radii randomly placed into space (see figure 1(a)). A special packing algorithm of collective rearrangement is used here in order to increase the maximum volume fraction computable in acceptable time [BEZ 02]. This method is extremly efficient when it comes to specific size repartition of aggregates. Only little work on the radii probabilistic distribution is required. Major drawback is the extremly simple spherical aspect.



(a) Sphere packing (b) Random field excursion set

Figure 1. *Morphological modelling using non-intersecting spheres packing or random fields.*

The idea behind the second method is to yield the phases using levet set of correlated random fields (see figure 1(b)). In opposition to white noises, the use of correlated random fields gives a spatial structure to the resulting morphologies (hereafter called excursion sets). A probabilist link between Gaussian correlated random field characteristics (mean, variance or correlation length) and both geometrical and topological quantities (volume, surface area, Euler characteristic...) has been recently made in [ADL 08], giving the possibility of controlling the excursion sets characteristics and applying it to represent each material phase and even make it evolve through time easily if needed, opening possibilities of hydration modelling problematics for instance. This method gives several advantages such has accurate control on each geometrical characteristics or representation of random shapes, but still makes it hard to yield high fraction volume disconnected morphologies. Yet, using Gaussian related random field (like the χ^2 field) and union of random fields allows to increase the fraction volume to reasonnable values.

Efforts of morphological modelling are here made within a multi-scale linear framework using a FE model with embedded discontinuities. In order to represent these heterogeneities, those morphologies are projected onto the FE mesh, thus defining a set of discontinuities within the strain field interpolation (weak discontinuities). These kinematics enhancements lead to "non-adapted" meshes in the sense of independence between heterogeneities morphology and the underlying FE mesh.

3. Finite Element failure modelling

The second main aspect of this work is about modelling the quasi-brittle behaviour of concrete-like materials. During the last decades, it has been shown that, in contrast to strain softening in classical continuum material models, allowing displacement discontinuities in the kinematics field leads to a more meaningfull description of the material nonlinear behaviour [SIM 93]. In the presented framework, discontinuities in the displacement field represent what we can call "meso-scale crack". In order to handle both heterogeneities and crack-opening mechanism at meso-scale, weak discontinuities are completed with a set of strong discontinuities within the framework of local enhancement [BEN 10]. The magnitude of the displacement discontinuity in each element gives the measure of the crack opening. Strong discontinuities are activated according to a certain localization criterion and are then governed by a simple relationship between traction vector and crack opening. Such elements are represented figure 2 from blue to red, regarding the magnitude of the crack. At a larger scale, the coalescence of several "local-cracks" shall represent the localization of a macroscopic crack. In other words, the local failure mechanism leads to global macroscopic failure by upscaling structural effect.

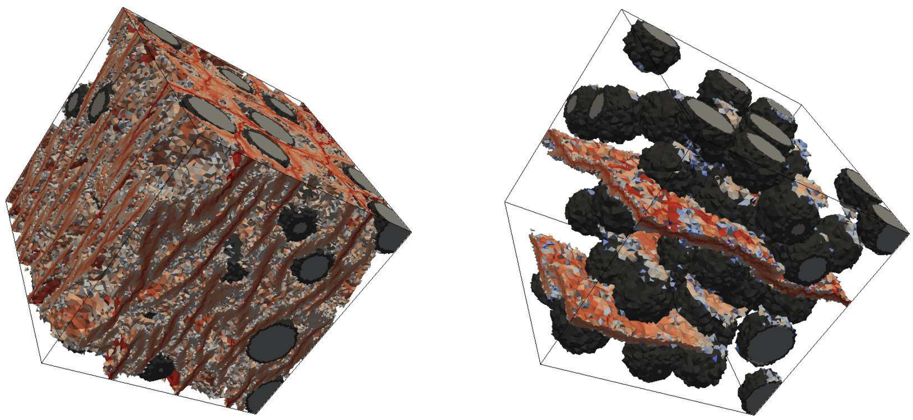
This vision of modelling the macroscopic behaviour by this natural method is the cornerstone of this work, leading to several original considerations. The main one is that this structural effect has a physical sense only if the mesoscale is physically well described. A simple tension/compression test presented in the next section point out the major effect of morphological description. However, by simulating a shrinkage mechanism, we show that adding an other kind of meso-scale description such has a pre-cracked pattern leads to more realistic macroscopic behaviour.

3.1. *Natural asymmetric tension/compression behaviour*

Results on both tension and compression simulations are presented here. They have to be seen has two completely independant calculations yet using exactly the same mesoscopic description in terms of morphology, material characteristics and mechanical behaviour. Hence, we show that very simple local failure mechanism are enough to retrieve much more complex features at macro-scale. For the two-phases material presented here (aggregates within a cement paste) three local desciptions are applied depending on whether an element is completely in the matrix, completely in an aggregate (in grey on figure 2) or in both (in black onfigure 2). The latter is called “interface element” and handles material discontinuities with special inherent enhancement, simulating a perfect interface. All the material characteristics are given in table 1. It is assumed that aggregates keep an elastic behaviour. On the other hand, after reaching a certain maximal stress in tension, maxtrix and interface element, by the mechanism of crack-opening dissipate a certain amount of energy before total failure. Hence, the tensile strength and the fracture energy are the two parameters governing the non linear behaviour.

	Young modulus $[MPa]$	Tensile strength $[MPa]$	Fracture energy $[J].[m]^{-2}$
Aggregate	80 000	–	–
Matrix	20 000	3	5
Interface	–	3	5

Table 1. *Material characteristics of the mesoscale*



(a) Macroscopic crack in compression test (b) Macroscopic crack in tension test

Figure 2. *Representation of the structural effect on the macroscopic crack for tension and compression test.*

A first comparison between the results of tension and compression tests can be made regarding the shape of the macroscopic crack (see figure 2). One can first notice that in both case, macroscopic cracks find their way around elastic aggregates leading to complex geometry and even “natural” branching. However, the global shape differs completly. When in tension, a single crack is well localized following a plan perpendicular to the solicitation, in compression, nearly all the elements are broken, leading to several plans, this time parallel to the solicitation. The differences observed between the macroscopic cracks reflect the asymmetric response of the material. All the upscaled mechanical characteristics of the material at the macroscopic scale are given table 2. Regarding the necessary energy to reach macroscopic failure we can note that both are bigger than the mesoscopic one, as it has been shown in experiments. Futhermore, those energies indicate that the behaviour in tension is way more brittle than in traction. Regarding the strength and the energy needed before total failure of the material, the difference between the two tests reflects the general more brittle behaviour of concrete-like material in tension than in compression.

	Young modulus $[MPa]$	Strength $[MPa]$	Fracture energy $[J].[m]^{-2}$
Tension	24 800	2	17
Compression	24 800	9	750

Table 2. *Upscaled material characteristic at macro-scale*

These simple tests show that, using the same mesoscopic description (mechanically and morphologically speaking), the upscaled macroscopic behaviour naturally represents a complex behaviour such as asymmetry between tension and compression response. The structural effect due to the perturbation of heterogeneities is the only reason of the asymmetric response observed. Yet several drawbacks can be noted regarding strength values. Both are rather low compared to reality, espacially the compression one. It can be improved with a more accurate morphological representation. Ideed, results presented herein are base on a monodisperse spherical method, yielding an aggregate phase of 20% fraction volume. Calculations (not presented here) have shown that increasing this volume by adding smaller balls (by following actual grrain size repartitions), or using random field excursion sets increase significantly the compression strength yet not much the tension one (increasing additionaly the strength ration).

3.2. *Effect of homogeneous shrinkage on the macroscopic response*

We saw that the outcome of the structural effect due to morphological representation brings strong asymmetric behaviour regarding tension and compression. In this section, we add to the simulation a homogeneous shrinkage mechanism by imposing a given strain, ε_{rd}, to the matrix before the tension or compression solicitation leading to a "pre-cracked" state of the material. Such homogeneous sollicitation can represent, for exemple, the effect of drying shrinkage incompatibilities between cement paste and aggregates [LAG 11]. It can be seen as a infinitly slow drying, leading to a diffuse crack pattern, in opposition to oriented one (that is the usual effect of differential drying [DESA 08]). The macroscopic response with (resp. without) shrinkage are shown figure 3 the dashed (resp. plain) curve representing the macroscopic reaction through the imposed displacement.

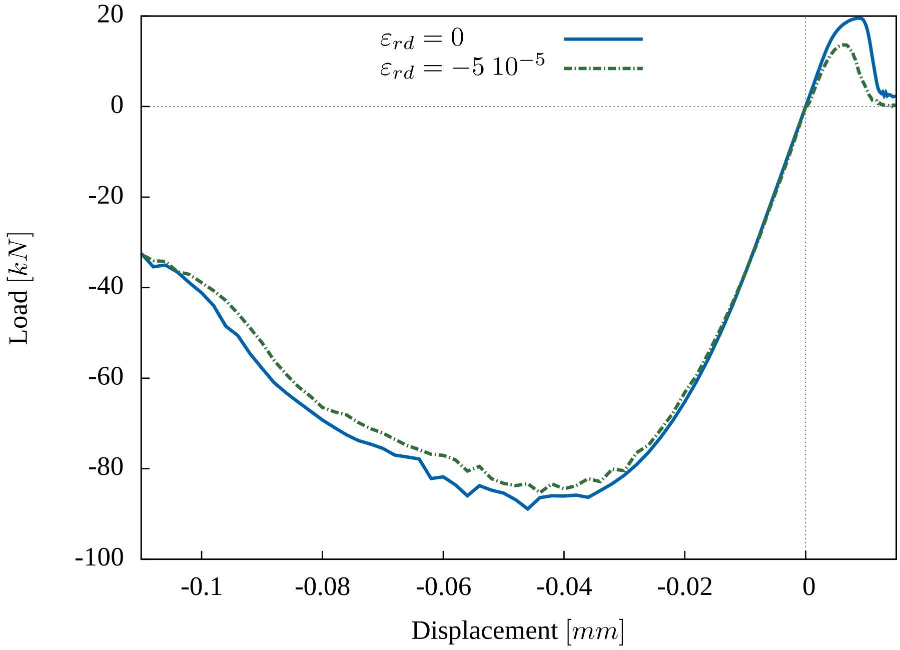


Figure 3. *Representation of the drying shrinkage mechanism on the macroscopic behaviour for tension and compression tests.*

		Young modulus $[MPa]$	Strength $[MPa]$	Fracture energy $[J].[m]^{-2}$
Tension	$\varepsilon_{rd} = 0$	24 800	2	17
	$\varepsilon_{rd} = 5\ 10^{-5}$	16 000	1.2	9
Compression	$\varepsilon_{rd} = 0$	24 800	9	750
	$\varepsilon_{rd} = 5\ 10^{-5}$	24 300	8.5	720

Table 3. *Upscaled material characteristic at macro-scale with drying*

We can note that the pre-cracked state has a more important effect in tension than in compression, leading to a bigger ratio between maximum stress in tension and in compression. The brittle behaviour of tension test is more sensitive to the shrinkage solicitation. It helps the localization of the one macroscopic crack leading to even more brittle behaviour. In opposition, the little effect it has on the compression response represents the higher complexity of the failure mechanism. However, the framework lacks mesoscopic physical effect modelling, leading to questionable results. For example, it as been shown that the increasing capillary tension due to shrinkage, increase the compression strength as well [SEL 09].

4. Conclusion

Most of problems related to concrete structures durability (such as reinforced concrete corrosion or delayed ettringite formation) are directly linked to mass transfers. Thus they are clearly affected by any mechanical degradation in the sense that any set of meso- or macro-cracks shall increase those transfers by several orders of magnitude. Here the detailed knowledge of the meso-scale cracks pattern (cracks openings and orientations) is a useful tool for such matter. For exemple, dealing with water or gaz permeability issues, a macroscopic crack in a material leads to strong anisotropy due to its orientation (figure 2) and linking it to a macroscopic permeability tensor is not an easy task. The knowledge of the crack provided by the framework presented here gives the basis of a new upscaling permeation scheme [JOU 11].

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