# The influence of aggregate shape, volume fraction and segregation on the performance of Self-Compacting Concrete : 3D modeling and simulation

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*RÉSUMÉ. Un Béton Auto-Plaçant (BAP) est un béton contenant un volume de pâte de ciment élevé, et coulant ainsi plus librement qu'un béton classique. Il peut, en conséquence, être utilisé pour former, sous son propre poids et sans vibration, des formes complexes. Toutefois cette fluidité élevée prédispose le Béton Auto-Plaçant à un risque plus élevé de ségrégation par rapport à un béton vibré, c'est-à-dire à une séparation entre la phase de mise en suspension et les granulats, ce qui peut avoir une incidence sur le comportement du matériau. Dans ce travail nous étudions le comportement mécanique du béton par le biais d'une modélisation 3D réaliste et morphologique pouvant considérer 3 phases distinctes : la matrice de mortier, les inclusions (granulats) et la zone de transition. Un comportement élasto-plastique endommageable est supposé pour la phase de mortier sous chargement quasi-statique. La modélisation est ensuite développée pour déterminer l'effet de la forme globale des inclusions, de la fraction granulaire, et de la ségrégation sur le comportement du béton sous chargement uni-axial.*

*ABSTRACT. A self-compacting concrete (SCC) is basically a concrete with a higher volume of cement paste, that flows more freely than conventional concrete and can, as a result, be formed into complex shapes under the effect of its own weight without shaking. However, this elevated fluidity predisposes SCCs to a higher risk of segregation compared to vibrated concrete, i.e. separation between the suspending phase and coarse aggregates, which can affect the mechanical behavior of the prepared concrete. In this work, we investigate the mechanical behavior of concrete using a realistic morphological 3D matrix-inclusion-ITZ model for concrete at the mesoscale. Assuming a compression damaged plasticity-based behavior for the mortar phase under quasi-static loading, the model is used to determine the effect of aggregate shape, volume fraction and segregation on the mechanical response of the concrete specimen under uniaxial loading.*

*MOTS-CLÉS : échelle-méso, béton, Voronoi, ségrégation*

*KEYWORDS: meso-scale, concrete, Voronoi, segregation*

## 1. Introduction

Concrete is essentially a heterogeneous brittle material that fractures through the formation, growth and coalescence of microcracks [NAG 05]. Failure processes in concrete depend on the loading rate and are signicantly influenced by micro-inertia of the material adjacent to a propagating microcrack and moisture in the capillary pores. Modelling of failure and fracture in concrete is one of the fundamental issues in structural mechanics.
These phenomena show that the mechanical response of concrete involves multiple length scales defined at various levels [PED 13]. The smallest length scale is associated with the microstructure (cement paste) composed of water, hydrates (C-S-H) and anhydrous cement grains. The meso-scale is divided into a sub-meso-scale where the mortar is considered to be constituted by sand particles embedded in a homogenous cement paste, and a meso-scale itself representing concrete as a two or three phase composite material (mortar matrix and aggregates with or without an Interfacial Transition Zone or ITZ).
A realistic numerical simulation of material behavior must adequately represent the influence of as many of these length scales as possible on the mechanical response. Purely macroscopic models that do not consider the mesoscale or microstructural interactions usually lose vital information, for example, in problems related to durability. Lattice models have been used with some success [SCH 97, CUS 03] but they appear to have a major drawback in that the results obtained show a strong dependence on the lattice geometry considered. On the other hand, a mesoscopic model based on a regularized continuum description using a two or three-phase composite model taking matrix-inclusion interaction into account, coupled with a regularized model for the bulk material, is an effective approach for the characterization of the effects of the different length scales on the mechanical behavior. These models also present an excellent compromise between the computational effort involved and reliability of the result obtained.
Mesoscopic modeling of concrete needs a sufficiently accurate morphological model for the mortar-aggregate composite. The mortar phase may be described as a partially saturated open porous medium. Aggregates in concrete are characterized by their mineralogical nature together with their morphology (shape) and granulometry (size distribution). These aggregates may be of different types (siliceous, plastic, calcareous) and having different textures (rough or smooth) [KAM 14] as a result having different levels of bonding to the mortar [KEI 14], and have an angular and elongated or rounded and compact shape, all of which can have a significant influence on the stress distribution within the concrete material [WRI 06] and thus contribute to differences in mechanical behavior of the final formed concrete. This means that in the generation of random concrete structures the shape of aggregate particles has to be taken into account in order to study the effect of aggregate shapes upon the mechanical behaviour of the composite. A survey of the existing literature shows numerous implementations of mesoscopic modeling of concrete, but there are issues related first to the issue of mesoscopic representation of concrete, as well as the strain softening behavior of the cement mortar. Most have focused on either 2D representations using either circles or polygons [ZAI 81, PED 13], and the papers involving a full bore 3D analysis have been limited mostly to spherical representations, arranged in a regular [KEI 14] or random fashion [BER 08, WRI 06, COM 09].
Numerical analysis of the thus-created heterogeneous materials using the FEM requires the discretisation of the created mesoscopic models. Different meshing techniques have been applied for the discretisation of complex microstructures including conforming and non-conforming meshes by using a projection of a uniform mesh into the heterogenous material, as well as cubic meshes with an increased number of integration points [ZOH 81].
Moreover, the heightened fluidity of SCCs predisposes them to a higher risk of segregation compared to vibrated concrete, i.e. separation between the suspending phase and coarse aggregates, which can affect the mechanical behavior of the prepared concrete. To the author's knowledge, there is very little existing quantitative research on the effect of aggregate segregation on the mesoscopic behavior of a concrete specimen.
The mechanical constitutive behavior of the cement mortar (strain softening) and the nature of interaction between the phases is another important element that can cause significant variation in the results obtained. Depending on the type of loading, either brittle failure or viscoelastic rate-dependent models are typically used, with a few implementations focusing on quasi-static displacement controlled loadings where plastic behavior may be observed.
In this contribution we will perform three-dimensional analyses of quasi-static compression and tension tests of a concrete specimen at the mesoscale level. We use a rate-independent isotropic inviscid plastic damage (CDP) continuum model to model the mechanical behavior of the matrix (mortar) under quasi-static loading in conjuction with an explicit morphological model for the meso-structure including aggregate grains (inclusions).
The effect of different aggregate shapes has been modeled using a random spherical representation as well as a series of non-intersecting randomly sized and oriented polytopes generated using an exploded Voronoi tesselation. In addition, the effect of aggregate segregation, a side-effect of using SCCs, has been taken into account in this mesoscale model.
The remainder of the paper is organized in the following manner : Section 2 explains the morphological three-

phase composite model used to describe concrete at the mesoscale. Section 3 explains the mechanical constitutive model used for the individual phases, Section 4 describes the experimental setup used to determine the mechanical constitutive parameters of the cement mortar used in the study, Section 5 provides the results obtained after simulation. The paper ends with concluding remarks and suggestions for future work.

## 2. Morphological model of concrete at the mesoscale level

An explicit morphological model has been developed for the mesostructure that considers the concrete specimen as a three-phase composite material (figure 1) :
In this material the matrix phase consists of the cement mortar, while the inclusions phase consists of the aggregate

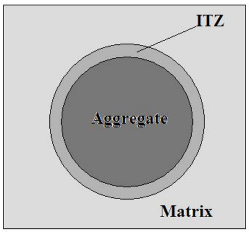


**Figure 1.** *Three-phase composite model of concrete*

grains, and the third phase is the interfacial transition zone (ITZ) for the cement paste, with a variety of contact conditions possible between the three phases.
In addition to these, the effect of aggregate segregation, a side-effect of using SCCs as has been explained earlier,

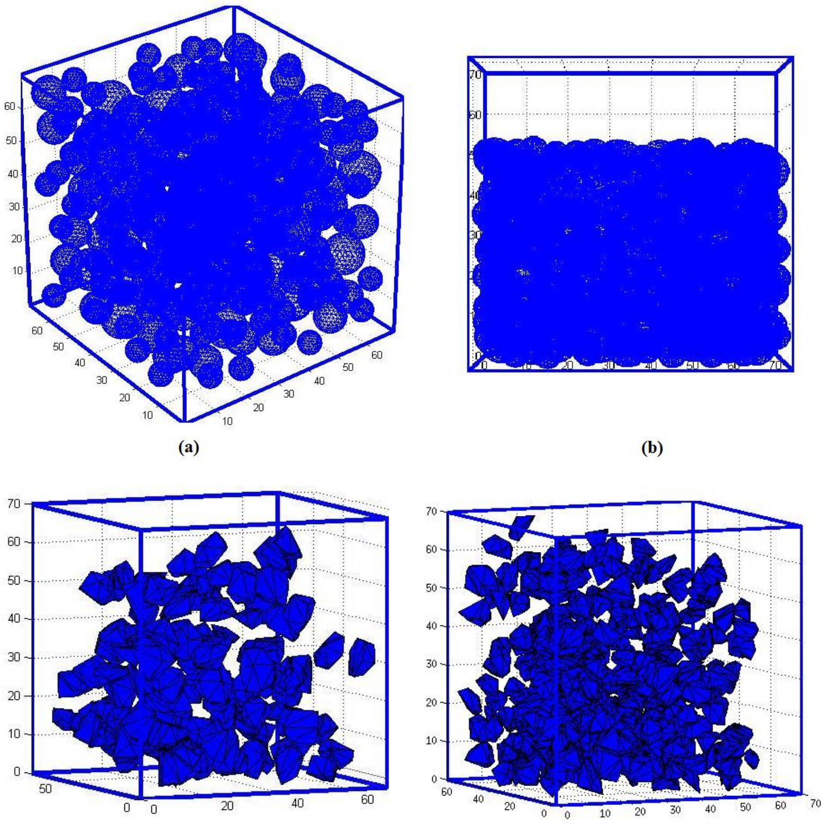


**Figure 2.** *Mesostructures with randomly packed spherical aggregates in* $7 \times 7 \times 7$ *concrete specimen (a) without and (b) with 25% segregation and polytopic aggregates at two different volume fractions in (c) and (d)*

has been factored into the mesoscale model as can be seen in figure 2 (top).

Figure 3 shows the FE meshes generated for both mesostructures (with spherical aggregates). Two kinds of aggregate shapes have been considered here : a random packing of spheres conforming to the desired granulometry and volume fraction represents the rounded aggregates, while a series of non-intersecting randomly sized and oriented polytopes satisfying the volume fraction and closely corresponding to the desired granulometry has been generated using an exploded 3D Voronoi tesselation along with a constraint the maximum number of vertices (15 in this work) as in figure 2 (bottom).
The corresponding FE mesh of the two phases as well as the ITZ phase of 200 $\mu m$ thickness is shown in figure 3.
All mesostructures have been obtained using our computational geometric modeling algorithm. For the spherical

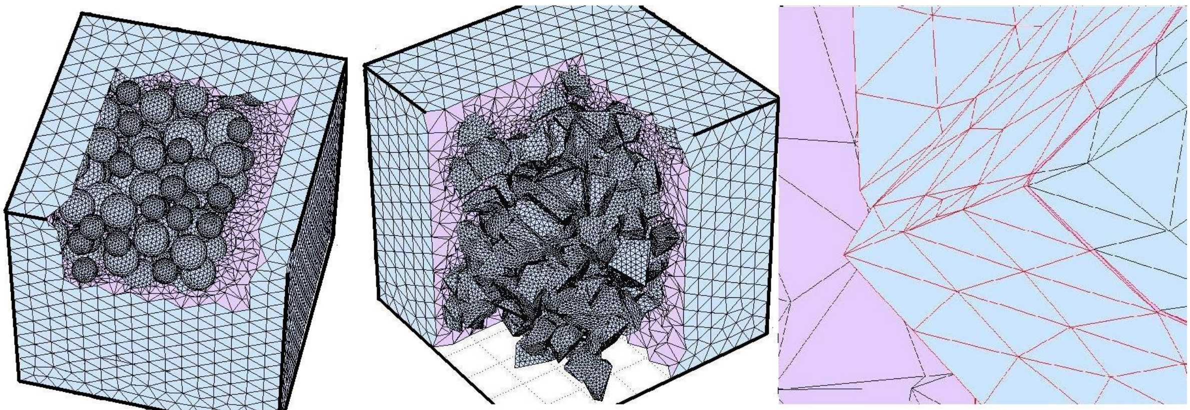


**Figure 3.** *(a) FE tetrahedral mesh for concrete specimen with polytopic aggregates generated by an exploded Voronoi tesselation (b) Zoomed in view of the Interfacial Transition Zone*

aggregates, we are able to achieve a random spherical packing that conforms exactly to both a given target volume fraction as well as a desired granulometry. Without segregation the packing algorithm attained a volume fraction of 27% within 25 seconds of CPU time. For the case of 25% segregated (along the specimen depth) spheres however, the same algorithm required 27 hours to achieve the target volume fraction of 27% and satisfy the chosen granulometric distribution. On the other hand, while the Voronoi packing (figure 3) is able to exactly satisfy the aggregate volume fraction constraint, it is extremely difficult to control the granulometry (size distribution) obtained. The advantage obviously is a realistic representation of the aggregate shapes.

## 3. Constitutive Models

### 3.1. *Phase I : Cement Mortar*

#### 3.1.1. *Mechanical behavior*

The main task in failure description is the recognition of damage patterns. Concrete Damage Plasticity (CDP) is a popular constitutive model that was introduced by Kachanov[KAC 58] and further developed by Rabotnov [RAB 71] and others, and has been used in this paper to describe the elasto-plastic mechanical behavior of the mortar phase. This model uses the concept of isotropic damaged elasticity in combination with isotropic tensile and compressive plasticity to represent the inelastic behaviour of the mortar.
In this model, the primary mode of failure in compressive loading is crushing while crack propagation is the primary mode of failure in tension, and the constitutive equation of mortar with scalar isotropic damage $d$ takes the following form :

$$\sigma = (1-d)\mathbf{D_0} : (\varepsilon - \varepsilon_\mathbf{0}) = (1-d)\bar{\sigma} \quad [1]$$

where $\bar{\sigma}$ is the effective stress tensor.
The scalar (isotropic) damage variable $d$ ($d = d_t$ in tension and $d_c$ in compressive loading respectively) is related to the equivalent plastic strain and the effective stress tensor :

$$d = d(\bar{\sigma}, \tilde{\varepsilon}^{pl}) \quad [2]$$

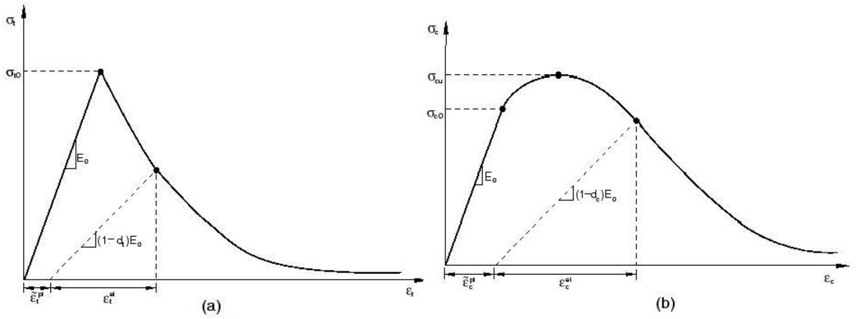

**Figure 4.** *Constitutive Behavior of Cement Mortar under uniaxial (a) compressive (b) tensile loading.*

Also, damage states in tension and compression are characterized independently by the equivalent plastic strains in tension and compression, $\tilde{\varepsilon}_t^{pl}$ and $\tilde{\varepsilon}_c^{pl}$ respectively. In terms of effective stresses, the yield function takes the form :

$$F(\bar{\sigma}, \tilde{\varepsilon}^{pl}) = \frac{1}{1-\alpha}\left(\bar{q} - 3\alpha\bar{p} + \beta(\tilde{\varepsilon}^{pl})\hat{\bar{\sigma}}_{max} + \gamma\hat{\bar{\sigma}}_{max}\right) - \bar{\sigma}_c(\tilde{\varepsilon}^{pl}) \qquad [3]$$

Failure via crack propagation (tension) and/or crushing (tension) is represented by increasing values of $\tilde{\varepsilon}_t^{pl}$ and $\tilde{\varepsilon}_c^{pl}$ respectively, which control the evolution of the yield surface as well as the degradation of the elastic stiffness of the mortar.
The concrete damaged plasticity model assumes nonassociated potential plastic flow. The fundamental group of the constitutive parameters consists of 4 values, which identify the shape of the flow potential surface and the yield surface. Considering the Drucker-Prager model for the flow function :

$$G = \sqrt{(R_c - mR_t tan\beta)^2 + \bar{q}^2} - \bar{p}.tan\beta \qquad [4]$$

where $R_t$ and $R_c$ are the uniaxial tensile and compressive strengths of concrete respectively. $\beta$ is the dilation angle measured in the $p - q$ plane at high confining pressure, $m$ is an eccentricity of the plastic potential surface, $\bar{p} = -\frac{1}{3}trace(\bar{\sigma})$ and $\bar{q} = \sqrt{\frac{3}{2}(\bar{\sigma} + \bar{p}) : (\bar{\sigma} + \bar{p})}$.
To identify these 4 constitutive parameters for the mechanical behavior mortar used in this work, the 3 standard laboratory tests were performed on a specimen, as described in section 2 : uniaxial compression, indirect uniaxial tension (Brazilian test) and triaxial compression.

### 3.2. *Phase II : Aggregates*

Aggregates in concrete may be siliceous, calcareous (limestone) or plastic in origin. Depending on the type of aggregate, we have different contact conditions between the matrix and inclusions. Limestone aggregates may be assumed to have a perfect contact with the surrounding mortar. Plastic aggregates may be assumed to have a frictionless sliding contact with the mortar.
In all cases, we may assume a linear-elastic-brittle behavior for the aggregates in the mechanical model.

### 3.3. *Phase III : Interfacial Transition Zone*

In the more general case, we need to consider the effect of a third phase, called the ITZ. This is generally an extension of the mortar phase, with the aggregates considered as embedded in the ITZ phase. For the simulations involving an ITZ, we have assumed perfect contact between the aggregates and the ITZ, as well as between the ITZ and the mortar phase. In this particular study, the ITZ has been assumed to have no influence on the overall compressive behavior of the concrete specimen [KEI 14].

## 4. Materials and Experimental Techniques

A standard displacement-controlled uniaxial compression test was performed on a specimen of mortar with the dimensions $40 \times 40 \times 160$ mm to obtain the elastic constitutuve and damage parameters for the mortar (figure 5).

This was then followed by compression tests on the two concrete specimens of size $70 \times 70 \times 70$ mm :
 the second one with a segregation of aggregates along 70% of the specimen's height for the same aggregate vo-


**Figure 5.** *(a) Concrete specimens* $70 \times 70 \times 280$ *mm with and (b) without aggregate segregation along the depth direction, (c) Experimental Set-up for the uniaxial compression test on specimens of mortar to obtain the mechanical behavior.*

lume fraction.

## 5. Results and Discussion

The results of the simulated quasi-static uniaxial compression tests for a $70 \times 70 \times 70$ mm concrete specimen containing various volume fractions of aggregates with the two different aggregate shapes described in the earlier sections are presented below. In all, 6 virtual tests were performed for the mesostructures in figure 2 - 4 for a specimen with polytopic aggregates at 20%,22%, 25% and 27% by volume respectively and 2 for a specimen with rounded (spherical) aggregates at 27% by volume with and without segregation - using tetrahedral FE meshes similar to those in figure 3.
The displacement-based compression test was controlled at a speed of 0.25 $\mu$m/sec and was carried out until failure of the specimen or excessive element distortion (which occurred in 2 of the 6 virtual tests).
The effect of aggregate segregation along 70% of the depth was the first effect to be modeled using the mesostructures shown in figure 2 using spherical inclusions (rounded aggregates) and the results are shown in figure 6. A slight increase in the UCS $\approx 3\%$ is obtained and is in agreement with experimental findings.
 Figure 7 shows the simulated distribution of the maximum principal strain inside the segregated specimen during the compression test, along and perpendicular to the direction of segregation. We see that when compressed along the direction of segregation the contours of maximum values for the maximum principal strain wrap around the contours with the aggregates throughout the sample, whereas when compressed along the perpendicular direction, the strains are localized in the zones containing the aggregates. The effect of aggregate shape was the second to be studied to compare the mechanical performance of a specimen with spherical inclusions (rounded aggregates) to the same specimen with the same aggregate volume fraction (27%) but with polytopic aggregates. The effect of aggregate volume fraction was then studied in order to evaluate the improvement/degradation in mechanical behavior with the addition of polytopic aggregates at different volume fractions, and the results are shown in figure 6.
These curves were then post-processed to obtain the results for the ultimate compressive strength and Young's modulus shown in figure 8. As expected, the Young's modulus increases in almost linear fashion with the aggregate fraction since the aggregates have a higher ridigity compared to the mortar.
 We expect the UCS to reduce with the aggregate volume fraction and this is indeed the case until a fraction of around 25% after which the UCS appears to improve. We could however chalk this up to a specific effect of the granulometry at this volume fraction, and would need a statistical analysis using a variety of granulometries and FE meshes to confirm this.

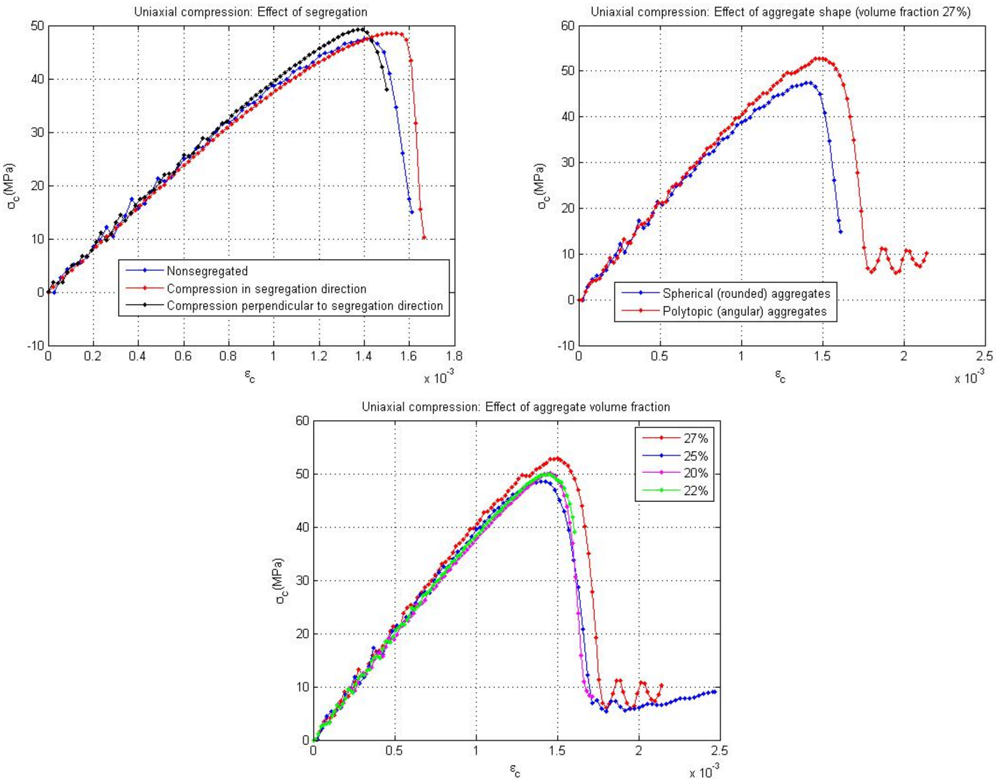


**Figure 6.** *Effect of aggregate segregation, shape and volume fraction on the compressive behaviour during a uniaxial compression test on* $70 \times 70 \times 70$ *mm concrete specimen.*

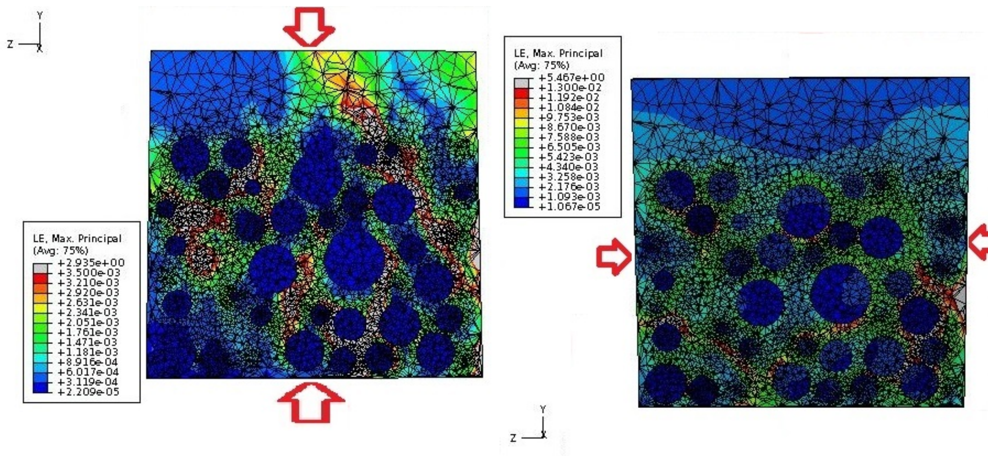


**Figure 7.** *Distribution of the maximum principal strain inside the* $70 \times 70 \times 70$ *mm concrete specimen for uniaxial compression (a) along and (b) perpendicular to the direction of aggregate segregation*

## Conclusions

In this work, we have described the development of a realistic morphological 3D matrix-inclusion-ITZ model for concrete at the mesoscale and used this model to perform a series of virtual tests on a concrete specimen, in order to characerize the mechanical behavior of concrete under quasi-static loading. We determined the effect of aggregate shape, volume fraction and segregation on the response of the concrete specimen. An obvious extension of this model is to study the hygral and hygro-mechanical coupling during autogenous and restrained shrinkage.

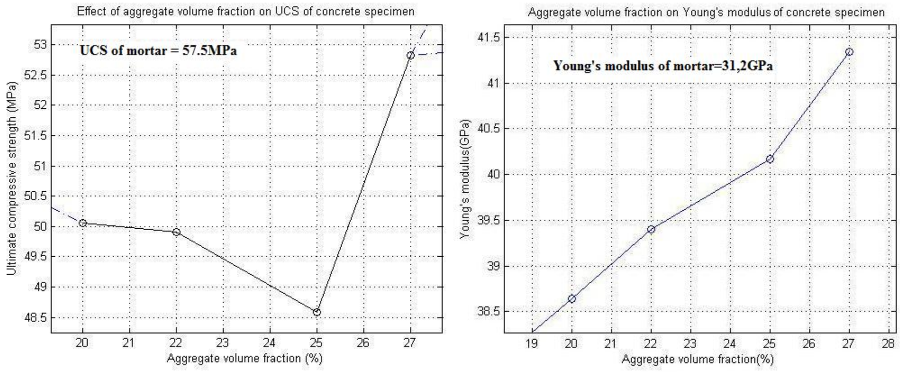


**Figure 8.** *Effect of aggregate volume fraction on UCS and Young's modulus of concrete assuming polytopic aggregates*

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