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EVALUATION OF THE LDPM ELASTIC AND FRACTURE PARAMETERS BY UP-SCALING PROCEDURE

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Abstract

The heterogeneity of the concrete may be considered on different size scales of observation, ranging from the atomistic scale (*$10^{-10}m$*), characterized by the behavior of crystalline particles of hydrated Portland cement, to the macroscopic scale (10^1m), where concrete has traditionally been considered homogeneous. The multiscale framework we are proposing in this paper is based on the following models: chemical analyses at the cement paste scale; mechanical lattice model at the cement and mortar scales; geometrical aggregate distribution models at the mortar and concrete scales; and the Lattice Discrete Particle Model (LDPM) at the concrete scale. For that purpose, a set of analysis starting from a known set of parameters of the cement paste. This input is utilized to evaluate the mechanical properties of the mortar-s (cement and sand), and then these properties are used to evaluate the mechanical properties of the mortar-a4 (mortar-s and aggregate smaller then 4mm). The upscaling in the proposed methodology involved the evaluation of the LDPM concrete parameters based on the mortar-a4 properties. Here we are suggesting a uni-axial tension "numerical experiments" on the mortar-a4 scale to evaluate the elastic and fracture LDPM mechanical parameters.

1. Introduction

Modeling the behavior of concrete structures is a challenging research task. Usually the mechanical behavior of concrete is macroscopically modeled via plastic and/or damage constitutive relations (e.g. see [1] among others). These macroscopic models are characterized by the large number of parameters needed to be calibrated in order to analyze the complex behavior of the concrete at the different stages of loading and at the different damage modes. The need of looking for alternative models for these macroscopic models is due to the fact that the concrete has a variety of microstructures. The variety of micro-structures includes: addition of fibers made up from different materials; variation of aggregate size, shape and type; water to cement ratio, cement composition, etc. The use of multi-scale analysis evidently is the appropriate way to model the behavior of concrete structures by coupling between the concrete micro-structures and its macroscopic properties needed to analyze a structure [2-17].

The microstructure of cement paste can be imaged either experimentally [18] or numerically [19-23]. Micro x-ray computed tomography (CT) [18] offers a nondestructive experimental technique to collect microstructure information of cement paste in terms of digitized voxels. Computer modeling packages are also available to simulate cement hydration and microstructure formation processes, including, the HYMOSTRUC3D model [19, 21], the CEMHYD3D [22], and the μic model [23].

The HYMOSTRUC3D model simulates the reaction process and the formation of the microstructure in hydrating Portland cement and takes into account the hydration kinetics. In this model, the cement particles are modeled as spheres, which grow during the hydration process. The HYMOSTRUC3D is designed as a 3D model by considering the water-to-cement ratio, the amount of cement, the mineralogical composition, cement fineness measured by Blaine apparatus, the temperature of the mix for Portland and blended cements, and specimen geometry as input parameters [24]. The Rosin–Rammler sieve curve is the approach adopted for describing the particle size distribution in the cement. The HYMOSTRUC3D model provides information concerning the location, morphology, and the degree of hydration of the cement particles. More details can be found in [19, 21].

The LDPM [2-10, 17] simulates concrete meso-structure by a three-dimensional assemblage of particles that are generated randomly according to a given grain size distribution. The approach usually adopted for the size distribution of the particles is the Fuller curve. The LDPM has been extensively calibrated and validated in the last few years, and it has shown superior capabilities from both qualitative and quantitative standpoints in reproducing and predicting concrete behavior under a wide range of loading conditions. The LDPM can simulate: 1) uniaxial (unconfined and confined) compression tests including the effect of specimen slenderness and the effect of friction of the loading platens; 2) biaxial compression tests; 3) triaxial compression tests with reversal of softening into hardening for increasing confinement; 4) hydrostatic compression tests, which never show softening; 5) direct tensile tests; 6) splitting tensile (Brazilian) tests; 7) fracture tests; 8) energetic size effects; 9) cycling loading; 10) the correct ratio between compressive strength and tensile strength; and 11) the rate effect on concrete strength. This model characterizes concrete at the meso-scale level—the level considered to be that of coarse aggregate pieces. This scale level takes into account the interaction between the various components of the concrete. The LDPM is formulated in the framework of discrete models for which the unknown displacement field is not continuous, but rather defined at discrete points representing the center of discrete particles. The geometric of the particles are obtained using Delaunay triangulation that provides volume subdivision into tetrahedral. The behavior of a particle contact represents the mechanical interaction between adjacent aggregate particles, through the embedding mortar. Such interactions are governed by meso-scale constitutive equations simulating meso-scale tensile fracturing with strain-softening, cohesive and frictional shearing, and nonlinear compressive behavior with strain-hardening. The contact areas are represented by the external triangular faces which are called facets. At the facet, the vectorial stress–strain relationships are imposed. Discrete compatibility equations are formulated through the relative displacements and rotations of adjacent aggregates (elements), where in each facet, there are two components for shear strains and a normal strain component. More details can be found in [7].

The goal of this research is to bridge between the microscopic cement paste scale and the concrete mesoscale by upscaling the cement properties in order to obtain the LDPM mechanical parameters. The proposed methodology is based on several models, as detailed in the nest sections, to provide the mechanical parameters of *mortar-4a* to obtain the input for the LDPM. As a result, the LDPM model will include information from the lower scales of the mortar constituents and might allow to reduce the number of experiments needed for the calibration process.

The LDPM was chosen to represent the concrete behavior at the meso scale level, due to its ability to capture the size, shape effects and the components influence of the concrete mix. The three lower scale models were chosen to provide the inputs of the 15 mechanical parameters of the LDPM are: The HYMOSTRUC model [19] for its capability to capture the information of mineralogical composition of cement clinker, the concrete mix proportion, and the chemical reaction of cement; The Anm material model [25] is used to simulate the concrete in meso-scale with irregular shape of aggregates and the lattice model suggested by [26] was chosen for its ability to simulate fracture process and the fact that this model has been validated with experiments [27]. This paper does not present validation study of the suggested numerical models as it already presented in [8], [30].

Finally, this paper suggests an upscaling of the elastic and fracture parameters of the LDPM using a successive analysis of three existing lower scale models.

2. Microstructure modeling of cement paste

In this research the (HYMOSTRUC3D) model suggested by [19], is used to simulate the cement hydration and microstructure of cement paste. The simulations were performed for a specific concrete mix design [28]. The microstructure of the cement paste is used for the further mechanical simulation of uniaxial compression to obtain the cement paste mechanical properties based on the specimen size, the mineralogical composition of cement, the cement fineness and the water/cement ratio. The concrete mix properties simulated in this paper are as follow: Portland cement (CEM 42.5 N/AM-SLV) with maximum cement size of *50 μm*, a w/c ratio of 0.567, air content 0.6 - 1.16% and the Iso and mix temperature of 20˚C. The w/c ratio of 0.567 was used for all scales (cement paste/mortar/concrete) simulations, due to the fact that all aggregates were saturated with dry surfaces and there are no superplasticizers in the mix. The mineralogical compositions of the cement were obtained from (XRD) analysis [27].The input parameters for HYMOSTRUC3D simulation are summarized in Table 1. The microstructures at the curing age of 3 hours are shown in Figure1 (left) and 28 days is shown in Figure1 (right).

The contour colors in Figure 1 represents the porous, unhydrated cement, inner hydration product, outer hydration product and CH.

Table 1: Specification of the HYMOSTRUC3D inputs used in the simulation

	Inputs specification
Mineralogical composition	C_3S: 54.9 %, C_2S: 19.1 %, C_3A: 4 %, C_4AF: 8.8%
Minimum particle diameter	1 μm
Cement fineness (Rosin-Rammler distribution)	(n = 1.05771, b = 0.04282)
Curing temperature	20°C

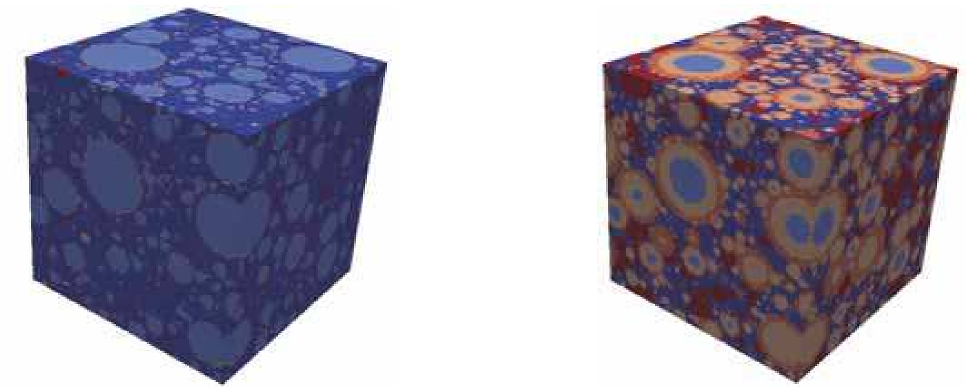

Figure 1: Microstructures of cement paste at –ages of 3 hours (left) and 28 days (right)

3. Mechanical simulation at, the microscopic scale

In order to evaluate the mechanical properties of the hydrated cement, 3D lattice model [26] is used to evaluate the mechanical properties of the cement paste at age of 28 days. The mechanical properties of each constituent of the microstructure are presented in Table 2 as published in [29]. In this scale we use a two-step homogenize presses as follow.

First homogenization step – at these step a thousand cubical specimens with size of 10μm×10μm×10μm were analyzed. Using uniaxial tensile test with (HF) – High Friction boundary condition were the lateral displacement is prevented at the boundary points and all other points are free to expand. The loading is imposing incrementally on the specimen as a unit displacement on the specimen in the longitudinal direction.

The lattice model converts the spherical particle that represents the microstructure of hydrated cement to a voxel-based digital image, where the ImgLat lattice construction method was applied, for more information see [29], in this paper the resolution is chosen to be 1 μm/Voxel. The mechanical properties required for the lattice model are the Young modulus, shear modulus, tensile strength and compression strength (the fracture energy of the cement is not included in the analysis of the used Lattice model) which are presented in Table 2.

Second homogenization step - at this step a cubical specimen size of 100μm×100μm×100μm were analyzed. The resulting stress-strain curve obtained from the simulation of the first homogenization step was approximated by a multi-linear curve. These multi-linear curves are the local mechanical properties of each element in this step depending on the location of each cube. A uniaxial tension simulation of this scale provides us the mechanical properties of the upper Mortar-s scale.

Table 2: Specification of the lattice model inputs used in the simulation of cement paste

No	Element type	Young modulus E (GPa)	Shear modulus G (GPa)	Tensile strength f_t (GPa)	Compression strength f_c (GPa)
1	Unhydrated cement	135	52	1.8	-1.8
2	Interface- Unhydrated & Inner	49	20	0.24	-2.4
3	Inner product	30	12	0.24	-2.4
4	Interface- Inner & Outer	25	10	0.15	-1. 5
5	Outer product	22	8.9	0.15	-1.5
6	Interface- Outer & CH	26.4	10.6	0.15	-1.5
7	(CH) - Calcium hydroxides	33	13.2	0.264	-2.64
8	Interface- Unhydrated & Outer	38	15.2	0.15	-1.5
9	Interface- Inner & CH	31.5	12.6	0.24	-2.4

4. Upscaling the Mortar-s scale

The Mortar-s scale includes cement paste, sand and interface transition zone. The mechanical properties of the sand and the interface between the sand and the cement paste are given in Table 3. The mechanical properties of the cement paste are given as multi-linear curve from the results obtained in section 3 as depicted in Figure 2. The specimen size chosen as $3mm \times 3mm \times 3mm$, in order to account for computational time and maintain reasonable results to consider the specimen as homogeneous [30]. The resolution of this scale needs to be equal or smaller than the cement specimen which was 100 µm × 100 µm × 100 µm, therefore the resolution is chosen to be 0.1 mm/Voxel, for more information see [29]. The mechanical properties required for the lattice model simulation are the Young modulus, shear modulus, tensile strength and compression strength which are presented in Table 3.

The performed simulation test obtained in order to provide results for the Mortar-a_4 scale is the uniaxial tension analysis as presented in Figure 3.

Table 3: Table Specification of the lattice model inputs used in the simulation of mortar s

No	Element type	Young modulus E (GPa)	Shear modulus G (GPa)	Tensile strength f_t (GPa)	Compression strength f_c (GPa)
1	Sand	70000	29000	24	-240
2	Interface- sand & cement	22000	8900	0.75	-7.5

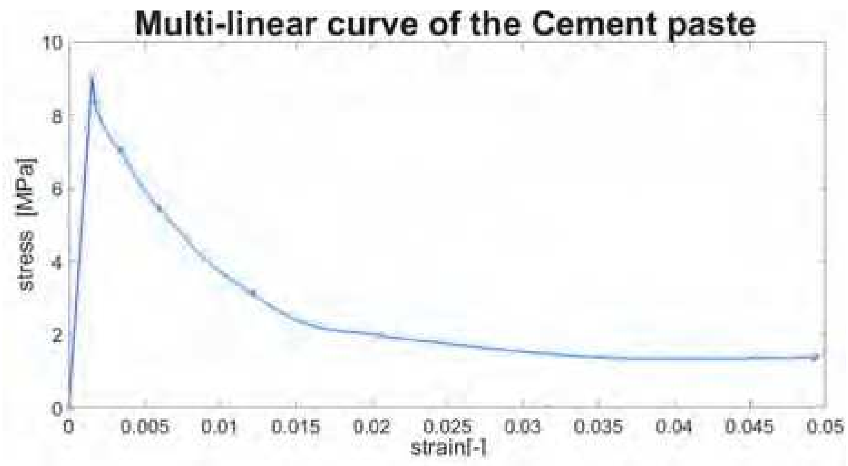

Figure 2: Cement paste stress-strain curve

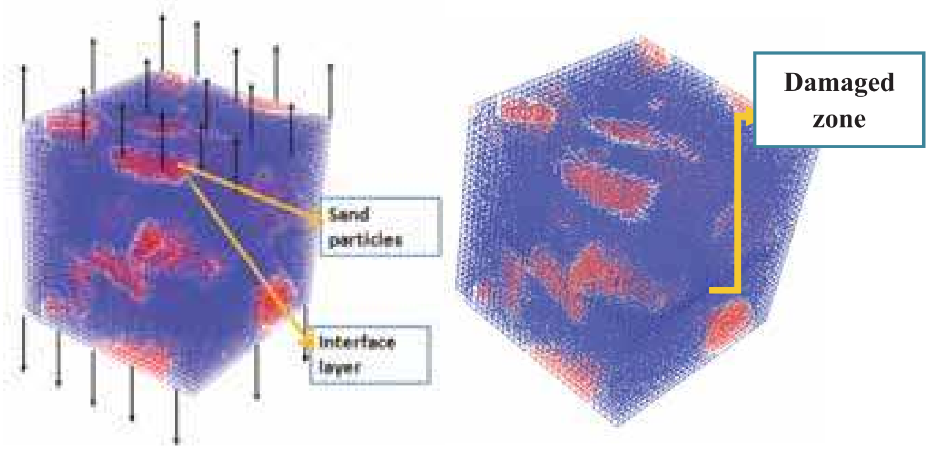

Figure 3: Uni-axial tension analysis on the Mortar-s scale and the resulted damaged zone on

5. Upscaling Mortar a_4 Scale

This scale represents the Mortar-a_4 which is the combination of Mortar-s, aggregates smaller then *4mm* and interface layer between them. From section 4 we obtain the Young modulus, shear modulus, tensile strength and compression strength of Mortar-s mechanical properties see Figure 4. To complete the mechanical information needed to analyze this scale the mechanical properties of the aggregates and the interface between the aggregates are given in Table 4. The specimen size chosen for this scale is $10mm \times 10mm \times 10mm$ and the resolution chosen to be 1 mm/Voxel. The Anm model has been applied to obtain the geometry of the mortar-a_4 unit cell. The Anm material model is used to distribute the aggregates particles into the unit cell with periodic morphology along the unit cell boundaries.

Table 4: Specification of the lattice model inputs used in the simulation of mortar a 4mm

No	Element type	Young modulus E (GPa)	Shear modulus G (GPa)	Tensile strength f_t (GPa)	Compression strength f_c (GPa)
1	aggregates	70000	29000	24	-240
2	Interface- aggregates & mortar s	41000	17000	1	-10

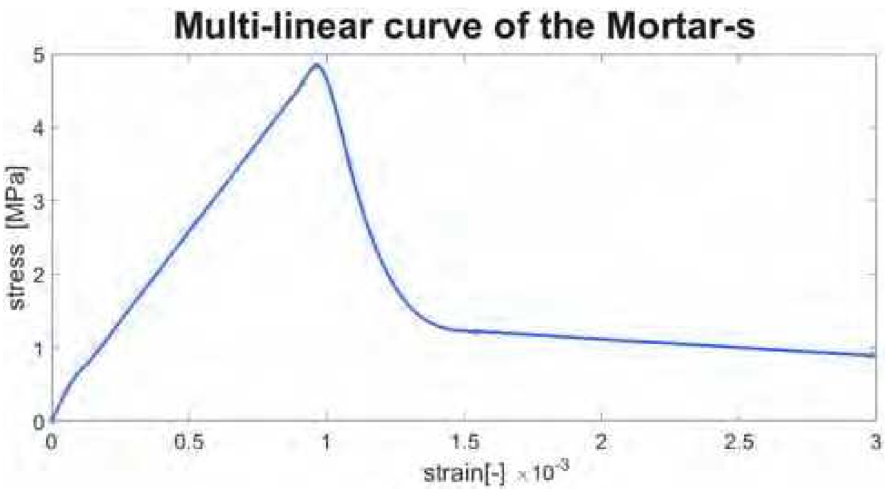

Figure 4: Mortar-s stress-strain curve

6. Evaluation of LDPM Elastic parameters

3D lattice simulations were performed at the *Mortar-a_4* scale in order to evaluate the elastic (E_0, ν), fracture (l_t, σ_t) and shear parameters for the LDPM. The LDPM constitutive parameters are representing the facet mechanical behavior where the mortar is located, therefore it can be assumed that the failure modes are characterized by the cement past up-scaled to mortar that includes aggregates smaller than *4* mm and ITZ (Interface Transition Zone). The simulation performed to evaluate these LDPM parameters are a uniaxial tensile test with High Friction (HF). HF boundary condition for the tension test were applied by preventing lateral displacement at the boundary nodes while all the other nodes were free to expand. The tensile simulation done by incrementally applying a displacement on the specimen in the longitudinal direction. As mentioned above the specimen size is *10mm×10mm×10mm* and the resolution chosen for this scale is *1mm*/Voxel.

The stress-strain curve of the Mortar-a_4 due to a tension simulation and the figures that relate the up-scaled LDPM parameters are presented in Figure 5. The pick value of the stress strain in Figure 5b is the tensile strength, σ_t, and it up-scaled directly to the LDPM as a material parameter. The fracture energy, G_t, can be calculated as the area under the stress–strain curve.

The fracture energy is calculated in order to define the characteristic length, LDPM parameter, as $l_t = \frac{2E_o G_t}{\sigma_t^2}$ see also Cusatis [7]. The normal elastic modulus, E_0, is calculated for each facet using the following expression $\frac{L}{E_0} = \frac{L_a}{E_a} + \frac{L_m}{E_m}$ where E_a and E_m are the module of elasticity and L_a and L_m are the length of the aggregate and mortar respectively, while L is the total length of the facet. The module elasticity of the mortar is evaluated from the slop of the stress-strain curve of the mortar (see Figure 5a), while the value of module elasticity of the aggregates are as published in the literature, e.g. see [29]. The Poisson ratio of the concrete is assumed as *0.18* and the LDPM α parameter is calculated as shown in Figure 5a.

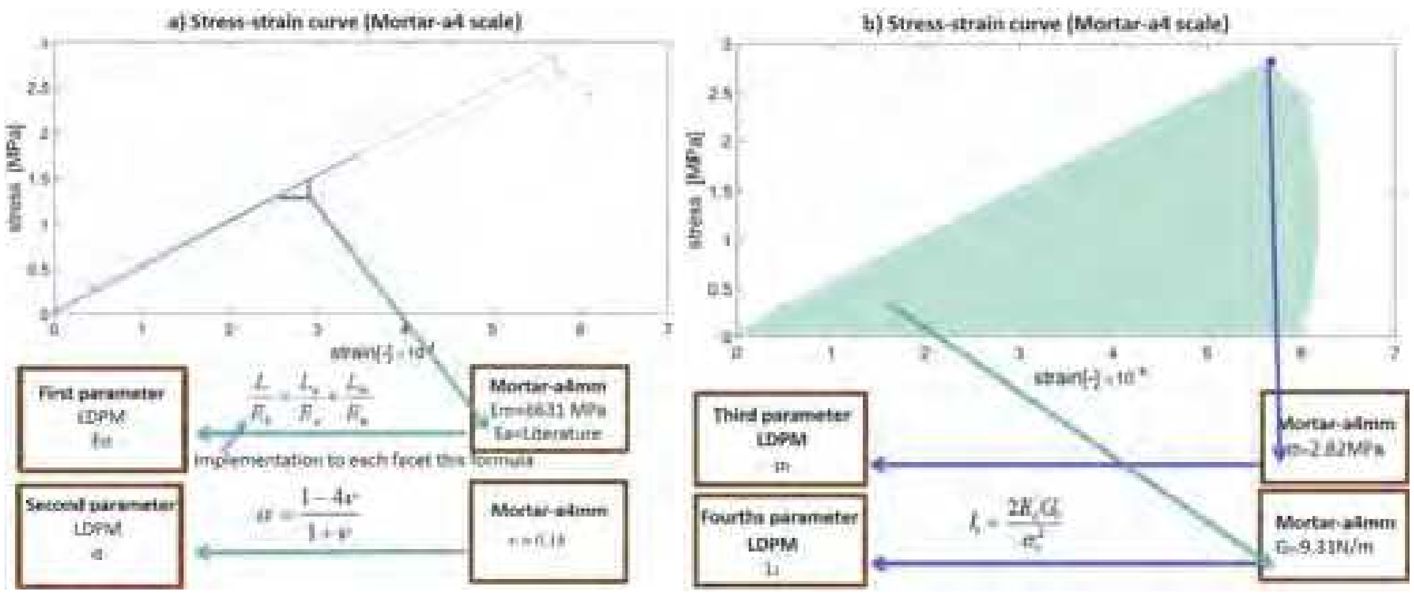

Figure 5: Mortar-a_4 stress-strain curve

7. Conclusion

The main aim of this research is to propose an upscaling procedure between the cement paste at micro-scale and the concrete at meso-scale, using existing models.

This research utilizes three models to obtain the parameters for the LDPM (concrete) model in order to obtain a full multi-scale technique that encompass all the various levels and take into account the contributory effects of lower-scale phenomena in the evaluation of the overall material properties at the macroscopic scale.

The three lower scale models that were chosen for the suggested upscaling procedure are: the HYMOSTRUC model for revealing cement hydration and microstructural formation, the Anm model for simulating the concrete in meso-scale with irregular shape of aggregates, and a lattice model based on Timoshenko beam elements for the mechanical analysis of the cement paste and the mortar scales.

The LDPM was chosen to simulate the concrete behavior at the meso-scale level, due to its ability to capture the size and shape effects and the effect of various concrete mix.

In this paper we demonstrated the suggested methodology by evaluating the elastic and fracture parameters of the LDPM.

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