Estimation of elastic properties of cement based materials at early age based on a combined numerical and analytical multiscale micromechanics approach

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ESTIMATION OF ELASTIC PROPERTIES OF CEMENT BASED MATERIALS AT EARLY AGE BASED ON A COMBINED NUMERICAL AND ANALYTICAL MULTISCALE MICROMECHANICS APPROACH

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Abstract

A multiscale approach based on analytical homogenization schemes combined with numerical homogenization is proposed. The analytical schemes are used to estimate the homogenized behaviour of cement paste and mortar. The numerical simulations are performed at the aggregate scale so that the effects of the form of the aggregate can be accurately evaluated. The scales of interest are the cement paste, the mortar (with the ITZ) and concrete (or coarse aggregate) scale. The cement paste and mortar are homogenized using generalized self-consistent and Mori-Tanaka schemes. Finally the concrete scale is assessed by finite element simulations with 3D generated microstructures where the aggregates consisting in polyhedrons obtained by a Voronoi space decomposition are randomly distributed in the mortar matrix.

1. INTRODUCTION

Concrete is a multiscale material, for which industrial applications demand a good description of macroscopic properties at the relevant scale of application. The elementary mechanisms modifying the properties of interest cannot generally be understood at that macroscopic scale and the resulting phenomenological approaches cannot a priori be extrapolated out of the domain in which the model was validated. From that emerges the importance of multi-scale approaches, which consist in the description of the mechanisms affecting the properties of interest at the microscale, and then linking the mechanisms through space scale in order to predict the properties at the scale of application.

Here, we focus on assessing the role of the aggregates in the mechanical behaviour of the structure but without neglecting the effects related to the other scales within the material. We are interested in the Young modulus and Poisson ratio, which evolutions are key parameters in the assessment of cracking in concrete at early ages [1].

A multiscale approach based on analytical homogenization schemes combined with numerical homogenization is proposed. The analytical schemes are used to estimate the homogenized behaviour of cement paste and mortar. The numerical simulations are performed at the aggregate scale so that the effects of the form of the aggregate can be properly evaluated. The scales of interest are:

– Cement paste composed of clinker minerals, hydration products and capillary porosity.
– Mortar composed of sand grains coated by an ITZ (Interface Transition Zone) layer and embedded in a homogenous cement paste matrix.
– Concrete (or aggregate) scale composed of aggregates embedded in a homogenous mortar matrix.

The cement paste and mortar are homogenized using the generalized self-consistent (GSCS) and Mori-Tanaka (MT) schemes. Finally the concrete scale is assessed by numerical simulations using the finite elements method with 3D generated microstructures.

2. ANALYTICAL HOMOGENEIZATION: CEMENT PASTE AND MORTAR

MT estimations for the bulk modulus k and shear modulus g are [2] [1]:

$$k^{MT} = \sum_p f_p\, k_p \left(1 + \alpha_0 \left(\frac{k_p}{k_0} - 1\right)\right)^{-1} / \sum_p f_p \left(1 + \alpha_0 \left(\frac{k_p}{k_0} - 1\right)\right)^{-1} \quad (1)$$

$$g^{MT} = \sum_p f_p\, g_p \left(1 + \beta_0 \left(\frac{g_p}{g_0} - 1\right)\right)^{-1} / \sum_p f_p \left(1 + \beta_0 \left(\frac{g_p}{g_0} - 1\right)\right)^{-1} \quad (2)$$

where f_p is the volume fraction of the phase p, with $p = 0$ refering to the phase considered as the reference medium (matrix) from which the parameters $\alpha_0 = 3k_0 / (3k_0 + 4g_0)$ and $\beta_0 = 6/5(k_0 + 2g_0)/(3k_0 + 4g_0)$ are obtained. MT estimations apply for microstructures exhibiting a pronounced matrix-inclusion morphology and take into account a certain level of interaction between particles [1]. GSCS estimations for the bulk modulus k of a $(n+1)$-coated sphere is [3]-[5]:

$$k_{n+1}^{GSCS} = k_{n+1} + \frac{f_n}{1 / \left(k_n^{hom} - k_{n+1}\right) + 3(1 - f_{n+1})/(3k_{n+1} + 4g_{n+1})} \quad (3)$$

where k_n^{hom} corresponds to the homogenized bulk modulus of the n-coated sphere and the volume fractions are computed with respect to the present phases regarding each layer. The GSCS estimation of the shear modulus can be determined from the equation [5]:

$$A\,(g_{n+1}^{GSCS})^2 + B\, g_{n+1}^{GSCS} + C = 0 \quad (4)$$

See [5] for the determination of the coefficients A, B and C. All the phases are assumed to be isotropic and homogeneous. The composite spheres own the same volume fraction for each of the elementary phases and occupy the entire volume of the material, which implies a distribution in their sizes ranging to the infinitesimally small [6]. Similar approaches were used to estimate both mechanical and transport properties of cement-based materials [6]-[8].

Here, we propose a combination of these schemes in order to predict the elastic properties of the mortar from the input of hydration balance.

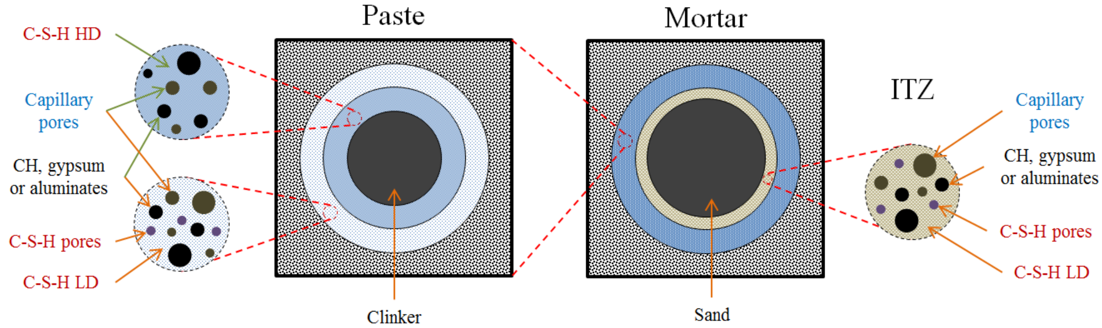

Figure 1. Schematic representation of the n-coated spheres representing cement paste and mortar

2.1. Cement paste

In order to estimate the elastic properties of the cement paste a 3-phases representation of the material is proposed (Figure 1). The core is composed of the cement grain coated by two coats. The first coat is composed of a fraction of the hydration products, water, empty pores and gypsum inclusions embedded in a matrix of *high density* C-S-H (C-S-H HD). The second coat is composed of a fraction of the hydration products, water, empty pores and gypsum inclusions embedded in a matrix of *low density* C-S-H (C-S-H LD). The elastic properties of the two heterogeneous coats are estimated with the MT scheme.

The volume fraction of reactants and products of hydration are determined from [9]. A kinetic model as the one developed in [10] may be used to estimate the evolution of the volume fraction as a function of time. The volume fractions within the cement paste and each coat for the composition presented in Table 1 are shown in Figure 2.

2.2. Mortar and ITZ

A 3-phase GSCS is used to estimate the elastic properties of the mortar (Figure 1). The core corresponds to the sand particle. We adopt the volume fraction of sand $f_{Sand} = 50\%$. The first coat is the ITZ and the second coat the homogenized cement paste.

We assumed that the ITZ is composed also of C-S-H LD and a part of the hydration products, water, gypsum and the empty pores from the cement paste. The part of the products and reactants going to the ITZ is discounted form the C-S-H LD coat. Experimental evidence shows that mortar and cement paste porosity presents different porosities [11]. We assume that this difference is due to the ITZ higher porosity compared to the cement paste [12]. Also, the ITZ is likely to contain more CH and A-phases [13]. These aspects are considered in the composition of the ITZ as shown in Figure 2.

2.3. Results

Using the values from Table 2, the Young modulus and the Poisson ratio obtained for the paste, mortar and ITZ are shown in Figure 3 and Figure 4, respectively. These results are consistent with experimental and modelling results for similar cement and w/c [1].

Table 1: Compositions from [14]

	C_3S	C_2S	C_3S	C_4AF	$C\hat{S}H_2$	w/c
Mass fraction	0.543	0.187	0.076	0.073	0.05*	0.5

**Assumed in this paper*

Table 2: Elastic properties of the different phases

	Clinker	C-S-H LD	C-S-H HD	CH	AFt	AFm	$C_3(A,F)H_6$	C_4AH_{13}	Gypsum	Sand
E [GPa]	140	21.7	29.4	38	22.4	42.3	22.4	25	45.7	74.5
ν	0.3	0.24	0.24	0.305	0.25	0.324	0.25	0.25	0.33	0.2
Ref.	[15]	[1]	[1]	[18]	[17]	[17]	[19]	[19]	[19]	[7]

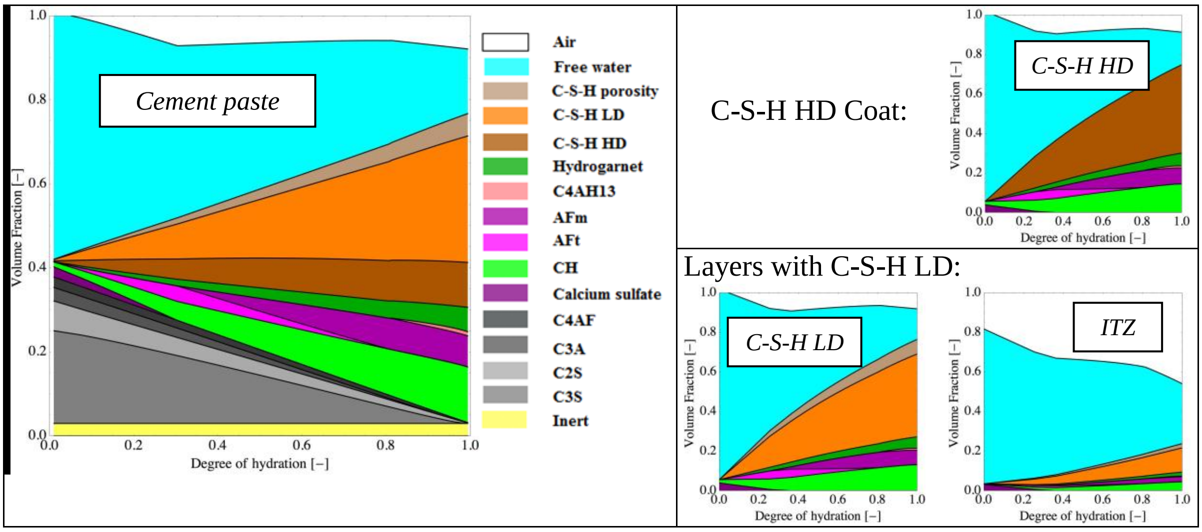

Figure 2. Volume fraction of the cement paste and different layers: C-S-H HD, C-S-H LD and ITZ

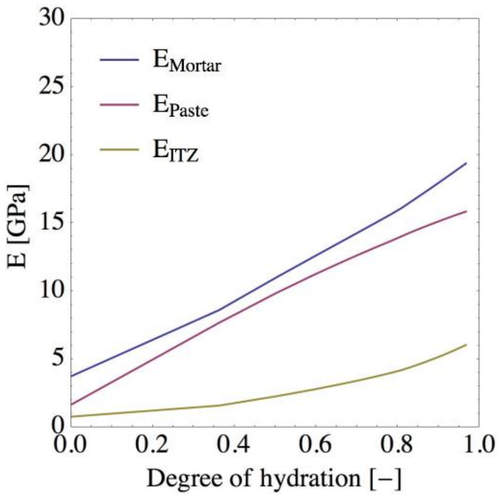

Figure 3. Young modulus of cement paste, mortar and ITZ

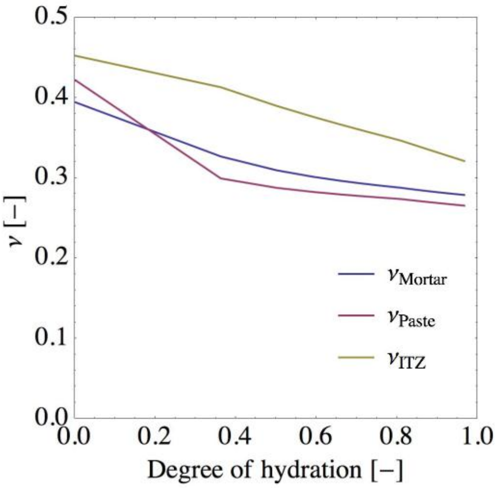

Figure 4. Poisson ratio of cement paste, mortar and ITZ

A similar tendency for the evolution of ν was found in [1] for the case in which the bulk modulus of the water was accounted for (k_{Water} = 2.18 GPa). A validation covering other w/c ratios and cement compositions are to be performed.

The estimation of E_{ITZ} remains in the range from 20 to 80% of E_{Mortar} [13]. Assuming that E_{Mortar}. is similar to $E_{Concrete}$, this result is in agreement with other results found in the literature [13]. With the GSCS estimate, it is assumed that the volume fraction of the external layer relative to the core one remains the same independently of the size of the particle. However it has been reported that the ITZ thickness remains nearly constant whatever the size of the aggregate [7]. In addition, because of the lack of data concerning the size and composition of the ITZ the results must be considered with reserves.

With the MT and GSCS estimations no percolation threshold is obtained. So the estimations for low degree of hydration may not correspond to the effective behaviour of the material.

These analytical results concerning the elastic properties of the mortar are used in the next section to estimate the behaviour of the concrete at the coarse aggregate scale.

3. NUMERICAL HOMOGENEIZATION: CONCRETE

The elastic behaviour of concrete at the mesoscale (coarse aggregate scale) is assessed numerically. The goal is to evaluate the influence of the form of the aggregate compared to the MT estimate for spherical particles at the concrete scale. Also, with a 3D numerical evaluation it is possible to assess locally the stress and strain distribution within the inclusions and the matrix.

3.1. Definition of the microstructure

The isotropic 3D generated microstructure in Figure 5 with 2.23 millions FE is used for the simulations. In this microstructure the aggregates consisting in polyhedrons obtained by a Voronoi space decomposition are randomly distributed in the mortar matrix consisting in a box of edge dimension of 120 mm. The total number of aggregates is 872with equivalent diameters varying between 8 and 18 mm. The same microstructures were used in the works [20] and [21]. The mortar properties are estimated analytically as presented in the previous section. For the coarse aggregates we adopt the volume fraction $f_{aggr} = 0.401$, E = 70 GPa and $\nu = 0.3$. The results are compared with the MT estimation (Eqs (1) and (2)) for concrete. Two boundary conditions associated with a uniaxial compression loading are considered: uniform stress (CLCH) and uniform strains (CLDHC).

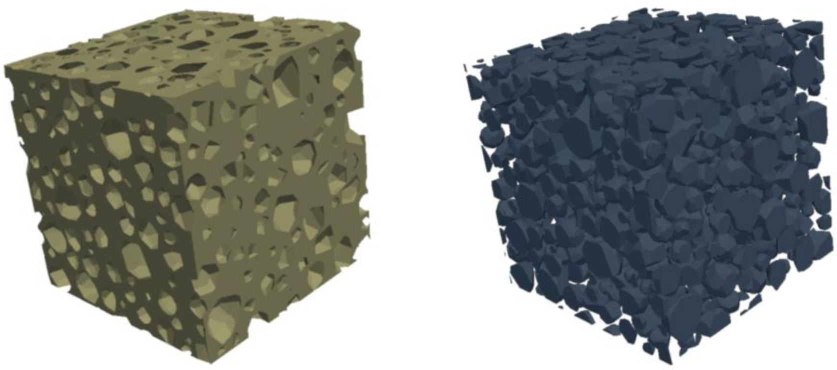

Figure 5. Microstructure: Mortar matrix (left) and coarse aggregate inclusions (right)

3.2. Results

The numerical estimations of the Young modulus and the Poisson ratio are compared to the MT estimate in Figure 6 and Figure 7, respectively. Both boundary conditions are shown. The results are in agreement with experimental results for similar concretes [1]. Due to higher contrasts between matrix and inclusions properties, the difference between numerical and analytical estimates is higher for lower degrees of hydration. On the other hand, for higher degrees of hydration the numerical and analytical estimates give close values.

The boundary conditions CLCH provide slightly better results than CLDHC. Because the matrix phase has here lower mechanical properties than the aggregate, this behaviour is expected [20].

The overall and average stresses within the matrix and inclusions in the direction of the applied loading σ_0 are shown in Figure 8. More dispersion in the values concerning the inclusions is observed, especially for low values of the degree of hydration. Similar tendencies are observed for the CLDHC boundary conditions.

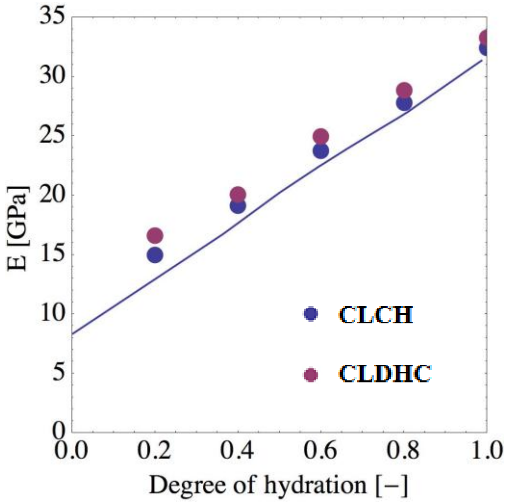

Figure 6. Young modulus of concrete: Numerical (dots) and MT (line)

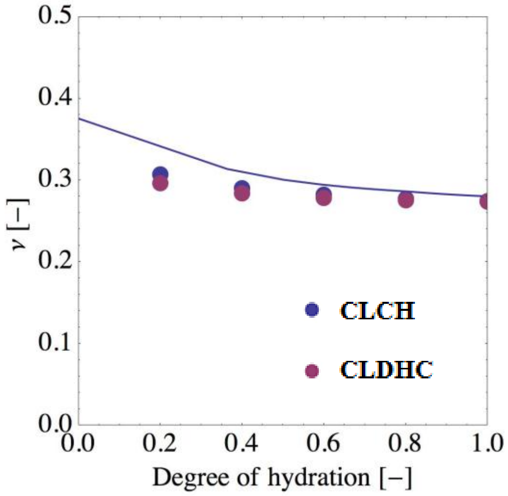

Figure 7. Poisson ratio of concrete: Numerical (dots) and MT (line)

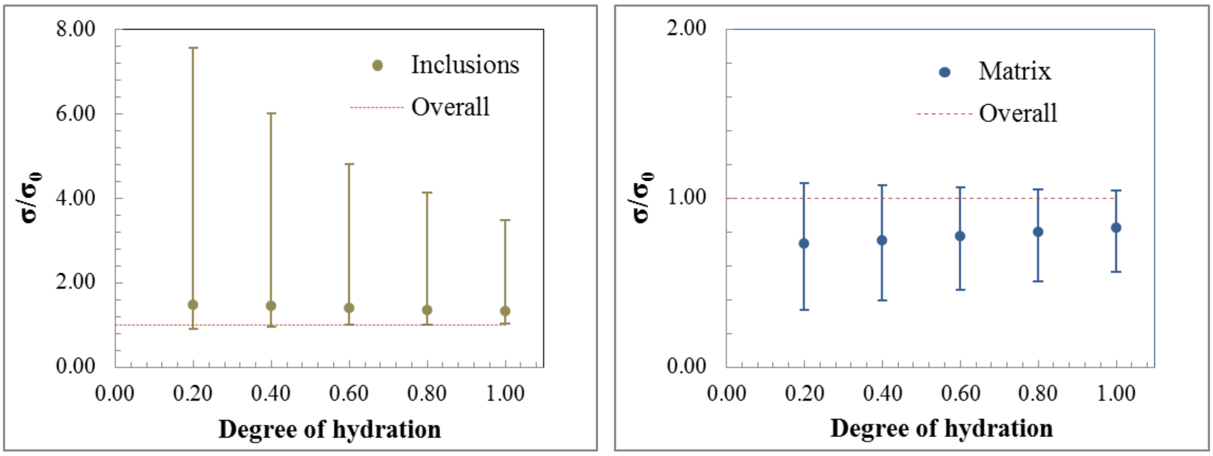

Figure 8. Overall stress and averaged stresses in the direction of the loading within the matrix and inclusions for CLCH: the dots indicates the averages stresses and the bar the maximum and the minimal values reached within the inclusions (left) and the matrix (right)

4. CONCLUSIONS

The results obtained are a first attempt in the estimation of elastic properties evolution at early age. This work provides a good basis for further developments including other aspects important for early age analysis, namely creep and shrinkage.

- The approach combining MT and GSCS schemes proposed here allows estimating the elastic properties of the mortar and the cement paste. Regarding the latter high density and low density C-S-H are accounted for. Regarding the former, the ITZ is considered. Such a formulation allows predicting the elastic properties from the composition of cement, paste and mortar. The influence of considering different LD and HD C-S-H and of the ITZ in the elastic properties can also be evaluated.
- As limitations, the analytical model is developed for spherical particles and does not present intrinsically a percolation threshold as observed experimentally for cement pastes. Also, the ITZ is assumed to have a uniform density and hydrates composition, which do not correspond to the experimental observations [7]. With the GSCS estimate, it is assumed that the relative volume fraction of the external layer and the core remains the same independently of the size of the particle. This seems not to be realistic regarding the ITZ. Further works are needed to investigate these aspects.
- The numerical estimations of the Young modulus and the Poisson ratio are in agreement with the usual values obtained experimentally for similar concretes. The numerical FE estimations are close to the MT estimate for higher degrees of hydration. Due to higher contrast between matrix and inclusions properties for low degrees of hydration, more important differences between the numerical and the analytical results are observed.
- As expected, uniform stress boundary conditions (CLCH) return better results than uniform strain boundary conditions (CLDHC), since the matrix phase has here lower mechanical properties than the aggregate. The stresses within the inclusions in the direction of the loading exhibit a significant dispersion, especially for low values of the degree of hydration.
- Further work will focus on the effects of the aggregates form (oblate and prolate) as well as the ageing viscoelastic behaviour of the matrix.

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