



Multiscale estimation of ageing viscoelastic properties of cement-based materials: A combined analytical and numerical approach to estimate the behaviour at early age



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ABSTRACT

We propose an investigation combining numerical and analytical tools to estimate the ageing viscoelastic properties of cement-based materials within a multiscale framework. With analytical homogenization the properties at the cement paste and mortar scales are estimated by a combination of Generalized Self-Consistent (GSC) and Mori–Tanaka (MT) schemes. With numerical homogenization the effective properties at the concrete scale are estimated. Numerical homogenization has the advantage of allowing assessing local information and to study more complex geometries. This combined strategy constitutes a promising tool to investigate how different mechanisms leading to ageing at the hydrated products scale, as well as other features of cement-based materials such as the Interfacial Transition Zone (ITZ), affect the viscoelastic behaviour at superior scales. In this context, we study the solidification of non-ageing constituents as the mechanisms leading to the ageing behaviour combined or not with a space-filling process in C–S–H. Relaxation and creep results are presented.

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1. Introduction

A relevant description of the behaviour of cement-based materials needs to account for the multiscale character of the material [1]. In general, industrial applications demand a good description of macroscopic properties at the relevant scale of application. However, the mechanisms modifying the properties of interest cannot generally be understood at that macroscopic scale. In the case of cement-based materials, these mechanisms occur at different time and space scales. For instance, regarding the specific case of viscoelastic behaviour of such materials, C–S–H behaviour is often reported to be linked to the origin of the viscous effects [2]. In this context, upscaling, or homogenization, techniques are interesting tools to understand and describe properly cement-based materials behaviour.

Using analytical homogenization, different properties of cement-based materials can be estimated at early and late ages. The elastic properties of concrete are estimated in e.g. [3–7]; the non-ageing linear viscoelastic properties at late ages can be upscaled by means of analytical techniques in Laplace–Carson space [8]. The ageing linear viscoelastic behaviour of concrete was less studied in a multiscale framework. Such constitutive behaviour seems to have been first studied by Maslov [9] to describe concrete behaviour [10]. The ageing character is

experimentally observed in Portland cement materials due to changes in the microstructure of the material which can be originated, for example, from the pursuit of hydration processes as well as relaxation of hydro-chemically induced self-equilibrated prestress of the microstructure [11,12]. Degradations processes (e.g. leaching), which can be coupled with the viscoelastic behaviour of the material itself, can be also a source of the ageing behaviour. In the following, we focus on the early age in which the hydration processes play a major role in the ageing aspect.

In this regard, Scheiner et al. [13] proposed an upscaling strategy using Mori–Tanaka (MT) and Self-Consistent schemes in Laplace–Carson space. Homogenization is applied at cement paste, mortar and concrete scales. The creep and relaxation tensors were obtained by numerical inversion of Laplace transforms. Then, the resulting ageing behaviour of the material was obtained by integration over the changes in the volume fraction of the constituents in time. The evolutions of the volume fraction are described by JMAK equations combined with a simplified description of the phases potentially present in the hydration processes. Another recent proposition in the direction of estimating the ageing linear viscoelastic behaviour of cement-based materials is made by Sanahuja [14]. Even if the full description of the scales of interest in cement-based material (from C–S–H up to concrete) is still not made, the author proposes a derivation of some classical homogenization schemes using formalism based on Volterra integral operator. This formalism allows establishing a correspondence between elasticity and ageing linear viscoelasticity [15,16]. Dilute, MT, Self-Consistent [14]

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and Generalized Self-Consistent (GSC) schemes [17] can be derived in an ageing linear viscoelastic framework in this way.

Correspondingly, using numerical homogenization, the elastic and non-ageing viscoelastic properties of concrete were estimated by different authors (see e.g. [18–23]) in studies of the long-term behaviour of concrete. Early-age investigations require a specific approach to deal with the evolution of the microstructure at the cement paste level. In this respect, the works involving the platforms μc [24,25], *CEMHYD* [26] and *Hymostruc* [27] are potentially leading-edge by allowing coupling hydration microstructure-based models with FEM (or other numerical methods) simulations to determine the effective properties of cement-based materials at early age. Once again, the ageing linear viscoelastic behaviour at early age was less studied. In this respect, for 2D mesostructures we highlight the works of Briffaut et al. [28]. Do et al. [25] estimated the ageing viscoelastic behaviour by means of FEM simulations with outputs of μc platform [24]; a scenario in which the space-filling intervenes in the C–S–H behaviour was studied by the author.

In this paper, we propose an investigation combining numerical and analytical tools to estimate the ageing viscoelastic properties of cement-based materials within a multiscale framework. With analytical homogenization the properties at the cement paste and mortar scale are estimated by a combination of GSC and MT schemes. With numerical homogenization the effective properties at the concrete scale are estimated. Numerical homogenization has the advantage of allowing to assess local information as well as to study more complex geometries. This combined strategy constitutes a promising tool to investigate how different mechanisms leading to ageing at the hydrated products scale, as well as other features of cement-based materials such as the Interfacial Transition Zone (ITZ), affect the viscoelastic behaviour at superior scales. Such strategy was previously used by the authors to estimate elastic properties [29] and ageing viscoelastic properties [30] of cement-based materials. Here, a more comprehensive and detailed analysis is provided regarding the latter case.

No effects of drying and temperature on the viscoelastic behaviour are considered in this paper. In other words, we are only dealing with basic creep and relaxation phenomena. Also, the discussion is focused on the early-age behaviour, so the mechanisms acting in the long-term behaviour are not accounted for. In the estimations presented in this work, we assume that a percolated structure exists at the different levels. At very early age this assumption is not true. This limits the scope of applicability of this work to periods after the percolation threshold.

2. Multiscale strategy

As mentioned in the Introduction, analytical homogenization is used to estimate the properties at the cement paste and mortar scale (Fig. 1). A two-coated sphere morphology is used to represent the cement paste and mortar microstructures [29,30], as proposed previously by e.g. [31, 32].

Regarding the cement paste, the hydrating particle is embedded in a high density (HD) products layer which is, in turn, embedded in a low density (LD) products layer. Following Bary and Béjaoui [31], we assume that the scale of these two subproblems is not the same since the typical size of the inclusions ranges from $<1 \mu\text{m}$ up to several tens of micrometre for massive crystals, whereas the characteristic length scale of C–S–H is 1 to 100 nm [33].

Regarding the mortar, the sand particle is embedded in an ITZ layer which is, in turn, embedded in a cement paste layer. The GSC scheme is used to obtain the homogenized properties of the cement paste and mortar. MT scheme is used to estimate the properties within each coat. The formulations of the schemes in ageing linear viscoelasticity are presented in Section 3.

Numerical homogenization is used to estimate the properties at the concrete scale. A specific procedure associated with the Finite Elements code Cast3M (<http://www-cast3m.cea.fr/>) to generate and compute 3D microstructures is used [34,35]. Local information regarding the stresses and strains repartition in the heterogeneities and in definite regions of the matrix are assessed. This is an advantage compared to analytical schemes that generally provide accurate estimations only on per phase averaged fields. With the local information, the zones in which stresses are localized can be more precisely identified. Previous results showed that a considerable dispersion of the averaged stresses within the inclusions and matrix subvolumes is observed [36].

3. Analytical homogenization: MT and GSC estimations

As previously mentioned, the derivation of the analytical homogenization schemes, needed in the proposed multiscale strategy, is performed in a specific ring in which Volterra correspondence principle (with respect to elasticity) holds [15,16]. With this correspondence principle the ageing linear viscoelastic behaviour can be upscaled.

In a set F of functions f , we define a ring $(F; +, \circ)$ in which the binary operator satisfies the conditions defining a division ring (or skew field), i.e. all nonzero elements have a multiplicative inverse but the

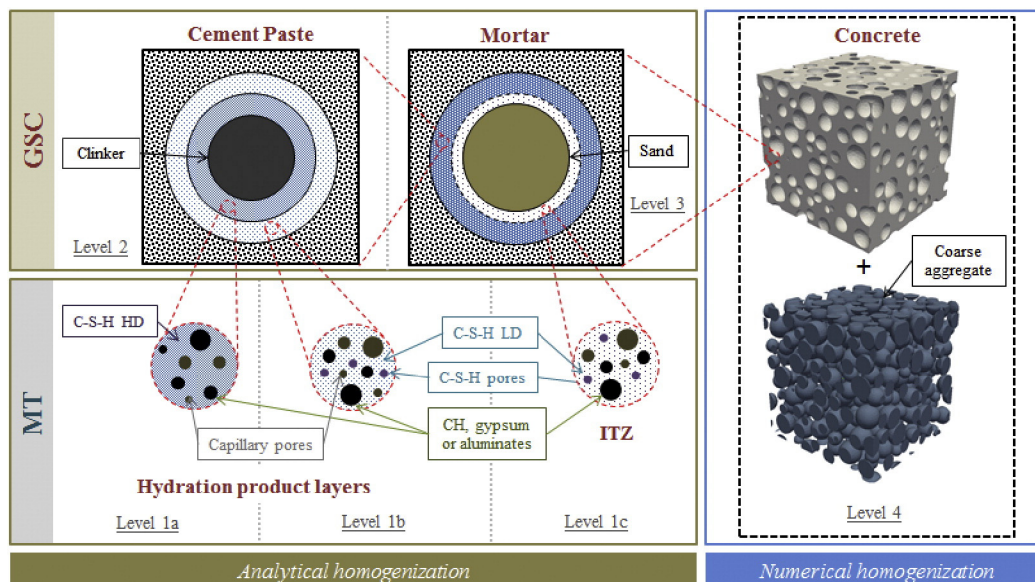


Fig. 1. Multiscale strategy with combined analytical and numerical homogenization.

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