



Upscaling quasi-brittle strength of cement paste and mortar: A multi-scale engineering mechanics model

Bernhard Pichler*, Christian Hellmich

Institute for Mechanics of Materials and Structures, Vienna University of Technology (TU Wien), Karlsplatz 13/202, A-1040 Vienna, Austria

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ABSTRACT

It is well known from experiments that the uniaxial compressive strength of cementitious materials depends linearly on the degree of hydration, once a critical hydration degree has been surpassed. It is less known about the microstructural material characteristics which drive this dependence, nor about the nature of the hydration degree–strength relationship before the aforementioned critical hydration degree is reached. In order to elucidate the latter issues, we here present a micromechanical explanation for the hydration degree–strength relationships of cement pastes and mortars covering a large range of compositions: Therefore, we envision, at a scale of fifteen to twenty microns, a hydrate foam (comprising spherical water and air phases, as well as needle-shaped hydrate phases oriented isotropically in all space directions), which, at a higher scale of several hundred microns, acts as a contiguous matrix in which cement grains are embedded as spherical clinker inclusions. Mortar is represented as a contiguous cement paste matrix with spherical sand grain inclusions. Failure of the most unfavorably stressed hydrate phase is associated with overall (quasi-brittle) failure of cement paste or mortar. After careful experimental validation, our modeling approach strongly suggests that it is the mixture- and hydration degree-dependent load transfer of overall, material sample-related, uniaxial compressive stress states down to deviatoric stress peaks within the hydrate phases triggering local failure, which determines the first nonlinear, and then linear dependence of quasi-brittle strength of cementitious materials on the degree of hydration.

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1. Introduction

Cement paste is the binder for cementitious materials, including cement mortar, concrete, shotcrete, and soilcrete. Therefore, a reliable prediction of mechanical properties of cement paste is paramount for subsequent modeling activities, be they related to material behavior of cementitious composites or to the structural behavior of engineering constructions built up from these materials. Challenging applications even require modeling of the evolution of mechanical properties of hydrating cementitious materials. This is e.g. the case for drill and blast tunneling according to the principles of the New Austrian Tunneling Method (NATM), where shotcrete tunnel shells are loaded by the inward moving rock, while the material still exhibits rather small maturities and undergoes the chemical hydration process. This provides the motivation for the present contribution which focuses on upscaling elasticity and strength of hydrating cement paste and mortar, by means of continuum micromechanics.

Within cement paste, hydration products (also called hydrates) establish the links that lead to a network of connected particles. The hydrates' non-spherical phase shape (evidenced by microscopic

[1–11] and neutron scattering [12] studies) has been recently shown to probably play an important role in micromechanics-based prediction of the quasi-brittle strength evolution of cementitious materials [13,14]. Thereby, hydration degrees have been estimated from elasticity measurements by means of a (validated) microelastic model, and corresponding measured strength values could be successfully predicted by a microelastic-brittle model with the hydration degrees as input. In this context, a mixture-invariant deviatoric hydrate strength was back-calculated. Having, in this way, gained confidence into the modeling approach, we here aim at a much stricter experimental model test: We wish to predict directly measured hydration-degree–strength relationships for different mixtures, with possibly avoiding any back-calculated strength values. Accordingly, the manuscript is structured as follows:

Section 2 recalls fundamentals of continuum micromechanics. In Section 3, we introduce a micromechanical representation of cement paste and mortar (Section 3.1), followed by corresponding mathematical expressions for upscaling elasticity (Section 3.2) and quasi-brittle strength (Section 3.3). Subsequently, we discuss model input values (Section 3.4). Therefore, we consider dense hydrate foams with very low porosity, from which we identify elastic properties that are, on average, representative for all hydration products. On this basis, our micromechanics models predict elasticity and strength of cement pastes and mortars as functions (i) of hydration degree and (ii) of

* Corresponding author. Tel.: +43 1 58801 20224; fax: +43 1 58801 9 20224.

E-mail address: Bernhard.Pichler@tuwien.ac.at (B. Pichler).

composition in terms of water-to-cement and sand-to-cement mass ratios (Section 3.5). Section 4 is devoted to model validation, based on the landmark experiments of Taplin [15] who measured early-age strength evolutions of hydrating cement pastes with water-to-cement mass ratios ranging from 0.157 to 0.8, as well as on the equivalence in strength evolutions of standard mortar defined in EN 196-1 [16] and of stoichiometric cement paste. In Section 5, we highlight general model characteristics related to uniaxial compressive strength of cement paste, as a function of the water-to-cement mass ratio and the hydration degree. Finally, we compare our elasto-brittle upscaling scheme with recently published ductile schemes related to the upscaling of confined hardness measurements on cement pastes and concretes (Section 6). This includes an estimate for the shear strength of hydrates.

2. Fundamentals of continuum micromechanics

2.1. Representative volume elements and separation of scales principle

In continuum micromechanics [17–20], a material is understood as a macro-homogeneous, but micro-heterogeneous body filling a representative volume element (RVE) with characteristic length ℓ . The separation of scales requirement implies (i) $\ell \gg d$, where d is standing for the characteristic length of inhomogeneities within the RVE, and (ii) $\ell \ll \mathcal{D}$, where \mathcal{D} stands for the characteristic lengths of dimensions or loading of a structure built up by the material defined on the RVE. Notably, “much smaller (\ll)” does not necessarily imply more than a factor of 4 to 5 between the characteristic length of the heterogeneities and that of the RVE [21].

In general, the microstructure within one RVE cannot be described in complete detail. Therefore, quasi-homogeneous subdomains with known physical quantities (such as volume fractions or elastic properties) are identified. They are called material phases. Once their mechanical behavior, their dosages within the RVE, their characteristic shapes, and the mode of their interactions are identified, the “homogenized” mechanical behavior of the overall material can be estimated, i.e. the relation between homogeneous deformations acting on the boundary of the RVE and resulting (average) stresses, or the ultimate stresses sustainable by the RVE, respectively.

In the framework of multiscale homogenization theory, a material phase, identified at a specific scale of observation “A”, exhibits a heterogeneous microstructure on a lower scale of observation “B”. The mechanical behavior of this microheterogeneous phase can be estimated by that of an RVE with a characteristic length being smaller than or equal to the characteristic length of the aforementioned phase, i.e. that of inhomogeneities identified on observation scale “A”, see, e.g. [22].

2.2. Field equations and boundary conditions

Within the volume Ω of an RVE, we consider field equations of linear elasticity, i.e. generalized Hooke's law accounting for linear elastic material behavior

$$\boldsymbol{\sigma}(\underline{x}) = \mathbb{C}(\underline{x}) : \boldsymbol{\varepsilon}(\underline{x}), \quad (1)$$

static equilibrium conditions (disregarding volume forces)

$$\text{div} \boldsymbol{\sigma}(\underline{x}) = 0, \quad (2)$$

and linear strain–displacement relations

$$\boldsymbol{\varepsilon}(\underline{x}) = \frac{1}{2} \left(\nabla \underline{\xi} + {}^t \nabla \underline{\xi} \right), \quad (3)$$

where \underline{x} denotes the position vector, $\boldsymbol{\sigma}$ and $\boldsymbol{\varepsilon}$, respectively, stand for the second-order tensors of stresses and strains, \mathbb{C} for the fourth-

order elastic stiffness tensor, and $\underline{\xi}$ for the displacement vector. The boundaries $\partial\Omega$ of the RVEs are subjected to linear displacements corresponding to a second-order strain tensor \mathbf{E} , i.e. we prescribe so-called Hashin boundary conditions [23], also referred to as uniform strain boundary conditions

$$\underline{\xi}(\underline{x}) = \mathbf{E} \cdot \underline{x}. \quad (4)$$

2.3. Homogenization of elasticity

The geometric compatibility of the microscopic strain field $\boldsymbol{\varepsilon}(\underline{x})$ with the uniform strain boundary condition (Eq. (4)) implies the following strain average rule

$$\mathbf{E} = \frac{1}{\Omega} \int_{\Omega} \boldsymbol{\varepsilon}(\underline{x}) dV = \sum_p f_p \boldsymbol{\varepsilon}_p, \quad (5)$$

where p denotes an index running over all phases of the considered RVE, $f_p = \Omega_p / \Omega$ stands for the volume fraction of phase p , and $\boldsymbol{\varepsilon}_p$ for the second-order tensor of average phase strains defined as

$$\boldsymbol{\varepsilon}_p = \frac{1}{\Omega_p} \int_{\Omega_p} \boldsymbol{\varepsilon}(\underline{x}) dV, \quad (6)$$

where Ω_p denotes the subvolume of the RVE occupied by phase p .

Analogously to Eq. (5), macroscopic stresses $\boldsymbol{\Sigma}$ are set equal to the spatial average of the equilibrated local stresses $\boldsymbol{\sigma}(\underline{x})$ inside the RVE,

$$\boldsymbol{\Sigma} = \frac{1}{\Omega} \int_{\Omega} \boldsymbol{\sigma}(\underline{x}) dV = \sum_p f_p \boldsymbol{\sigma}_p, \quad (7)$$

with $\boldsymbol{\sigma}_p$ as the second-order tensor of average phase stresses, defined by analogy to Eq. (6).

Linearity of the field Eqs. (1)–(3) implies a linear strain concentration rule

$$\boldsymbol{\varepsilon}_p = \mathbb{A}_p : \mathbf{E}, \quad (8)$$

with \mathbb{A}_p as the fourth-order strain concentration tensor of phase p . Specification of the elastic constitutive law of phase p

$$\boldsymbol{\sigma}_p = \mathbb{C}_p : \boldsymbol{\varepsilon}_p, \quad (9)$$

for the strain concentration rule (Eq. (8)) and insertion of the resulting expression for the phase stresses $\boldsymbol{\sigma}_p$ into the stress average rule (Eq. (7)) delivers a relation between macrostress $\boldsymbol{\Sigma}$ and macrostrain \mathbf{E} . Comparison of this relation with the macroscopic elastic law $\boldsymbol{\Sigma} = \mathbb{C}^{hom} : \mathbf{E}$ allows for identification of the homogenized elasticity tensor as [17]

$$\mathbb{C}^{hom} = \sum_p f_p \mathbb{C}_p : \mathbb{A}_p. \quad (10)$$

Knowledge of phase strain concentration tensors \mathbb{A}_p opens the door to scale transitions, i.e. it allows for computing average phase strains $\boldsymbol{\varepsilon}_p$ from the macroscopically imposed RVE-strain \mathbf{E} , see Eq. (8), and it permits homogenization (upscaling) of phase stiffnesses \mathbb{C}_p to the homogenized elasticity tensor of the RVE, \mathbb{C}^{hom} , see Eq. (10). As a rule, the concentration tensors \mathbb{A}_p are not known up to analytical precision. Still, they can be estimated based

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