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Micromechanical multiscale fracture model for compressive strength of blended cement pastes

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ABSTRACT

The evolution of compressive strength belongs to the most fundamental properties of cement paste. Driven by an increasing demand for clinker substitution, the paper presents a new four-level micromechanical model for the prediction of compressive strength of blended cement pastes. The model assumes that the paste compressive strength is governed by apparent tensile strength of the C-S-H globule. The multiscale model takes into account the volume fractions of relevant chemical phases and encompasses a spatial gradient of C-S-H between individual grains. The presence of capillary pores, the C-S-H spatial gradient, clinker minerals, SCMs, other hydration products, and air further decrease compressive strength. Calibration on 95 experimental compressive strength values shows that the apparent tensile strength of the C-S-H globule yields approx. 320 MPa. Sensitivity analysis reveals that the "C-S-H/space" ratio, followed by entrapped or entrained air and the spatial gradient of C-S-H, have the largest influence on compressive strength.

1. Introduction

Compressive strength of concrete and its evolution belong to the most important and tested parameters. Due to the multiscale nature of concrete spanning the range from sub-nanometers to meters and its composite nature, several factors on different scales play a role in concrete compressive strength [1]. The most relevant initial factors include the binder type, aggregate type, extent of the interfacial transition zone, and the air content. Time-dependent factors play a role mainly in binder's reaction kinetics which is reflected in the evolution of chemical phases with a direct impact on stiffness and strength evolution.

Up to the time of Hoover Dam construction in the 1930s, a cementitious binder was mostly equivalent to Portland cement. Since that time, Portland clinker has been substituted more and more by supplementary cementitious materials such as slag, fly ash, limestone or silica fume. The substitution rose from 17% in 1990 to 25% in 2010 among the top world cement producers [2]. A further shift is expected, motivated by economical, ecological and sustainable benefits [3,4].

The question on the origin of concrete strength becomes reinitiated with the advent of blended binders. The famous Powers' empirical relationship between the gel-space ratio and compressive strength developed for Portland-based materials needs several adjustments when dealing with blended binders [5]. The main reason lies in altered chemistry where a chemically heterogeneous gel differs in chemical phases, e.g. CH may be depleted in pozzolanic reactions or C-A-H phases may emerge. To overcome these deficiencies, micromechanical models taking into account volume fractions directly have been set up for more fundamental understanding.

Continuum micromechanical models able to reproduce the evolution of stiffness and compressive strength have recently been published, e.g. for Portland-based materials [6,7] or for cocciopesto mortars [8]. Pichler et al. [9] used spherical and acicular representation of hydrates to capture percolation threshold during hydration and the onset on elasticity and strength. Hydrates consisted of solid C-S-H, small and large gel pores and other hydration products. The strength criterion was based on deviatoric strength of hydrates which was identified to be 69.9 MPa. Once the quadratic stress average in arbitrarily oriented needle-shaped hydrates exceeded this strength, the material failed in a brittle manner. Similar modeling approach was also used for C_3S, C_2S, $C_3S + C_3A +$ gypsum pastes, assuming that only C-S-H with the Mohr–Coulomb quasi-brittle failure criterion was responsible for the compressive strength of pastes [10]. Computational micromechanical models generally allow taking into account nonlinear elasto-plasto-damage constitutive laws at the expense of computational time. Several 2D and 3D lattice and continuum models were applied for cement paste [11] or concrete [12,13,14] to mention a few.

In this paper, a new four-level micromechanical fracture model for blended cement pastes is presented, starting from C-S-H globule up to cement paste with entrapped/entrained air. The lowest homogenization

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level contains C-S-H globules, small and large gel pores [15]. A C-S-H globule is considered to be the only strain-softening component in the multiscale model, leading essentially to failure at each level. Softening occurs under excessive tension or compression described by an elasto-damage constitutive law introduced in Section 2.1. Higher levels also use the elasto-damage constitutive law for a phase containing C-S-H globules with an updated homogenized stiffness, strength, and estimated fracture energy. Hence, the strength of cement paste origins from the softening and failure of C-S-H globule. The multiscale model accounts for volume fractions of C-S-H, other hydrates, capillary porosity, clinker, supplementary cementitious materials, entrained/entrapped air and considers the spatial gradient of C-S-H among clinker grains.

The model contains two independent variables that need to be calibrated from experimental data: the apparent tensile strength of C-S-H globules and the spatial gradient of C-S-H. Numerical results for elastic modulus and compressive/tensile strength on each scale are further fitted to microstructure-calibrated analytical expressions, speeding up the whole validation part. Sensitivity analysis identifies key components for the compressive strength of blended pastes.

2. Finite element analysis

2.1. Fracture material model and its implementation

The nonlinear constitutive behavior of quasi-brittle materials, such as cement paste, mortar or concrete, can be generally described by three common theories: plasticity, fracture mechanics, damage mechanics, or their combinations. Plasticity fails to describe stiffness degradation which is needed for strain softening, strain localization, and the size effect, although several extensions were proposed [16]. Linear elastic fracture mechanics can only deal with brittle materials with a negligible process zone ahead of a crack tip and cannot handle microcrack nucleation into a macrocrack. Damage mechanics, particularly the cohesive crack model, defines the traction–separation law in a plastic zone of an opening crack which is related to the fracture energy of a material and stiffness degradation. This nonlinear fracture mechanics approach offers reasonable stress–strain predictions with minimum parameters, reasonable computation time, and captures the size effect of quasibrittle materials [17]. More elaborated plastic-damage models have been successfully used for the mesoscale analysis of concrete [14].

The present material model is based on fracture mechanics on all considered four scales. A crack starts to grow when cohesive stress is exceeded anywhere in the material. For uniaxial tension of a homogeneous material, this cohesive stress corresponds obviously to the tensile strength, f_t. Damage mechanics uses the concept of the equivalent strain, $\tilde{\varepsilon}$, as a descriptor of damage evolution. Damage becomes initiated when the equivalent strain, $\tilde{\varepsilon}$, exceeds strain at the onset of cracking, $\varepsilon_0 = f_t/E$, where E is the elastic modulus. The Rankine criterion for tensile failure defines $\tilde{\varepsilon}$ as

$$\tilde{\varepsilon} = \frac{\sigma_1}{E}, \sigma_1 > 0 \tag{1}$$

where σ_1 is the maximum positive effective principal stress on undamaged-like material, see Fig. 1 (a).

Under uniaxial compressive stress, crack initiation occurs under a different mechanism. A homogeneous material experiences only one negative principal stress and the deviatoric stress. Cracking in diagonal, shear band zone is often encountered on cementitious specimens, however, the physical mechanism is again tensile microcracking in voids and defects of the underlying microstructure [pp 297, 17]. Such a behavior has already been described in the work of Griffith [18], and McClintock and Walsh [19], and we briefly review this theory and extend it with an equivalent strain to be used in the framework of damage mechanics.

It is assumed that a material contains randomly oriented 2D elliptical flat voids with various aspect ratios $m = b/a$, see Fig. 1 (b). Further notations assume that tensile stress is positive and $\sigma_1 \geq \sigma_3$. The voids have a negligible area and only represent stress concentrators and internal defects in a material. Under macroscopic biaxial stress, the maximum tensile stress among all voids, $m \cdot \sigma_\eta$, appears on a critically inclined elliptical void under a critical angle ψ

$$\cos 2\psi = \frac{\sigma_3 - \sigma_1}{2(\sigma_3 + \sigma_1)}, \frac{\sigma_1}{\sigma_3} \geq -\frac{1}{3} \tag{2}$$

$$m \cdot \sigma_\eta = \frac{-(\sigma_1 - \sigma_3)^2}{4(\sigma_1 + \sigma_3)} \tag{3}$$

Crack formation occurs when the tangential tensile stress, $m \cdot \sigma_\eta$, equals to the tensile strength of the matrix. Since σ_η and the crack geometry, m, cannot be measured directly, it is reasonable to relate their product to the uniaxial macroscopic tensile stress, $\bar{\sigma}_1$, as proposed by Griffith [18]

$$\bar{\sigma}_1 = \frac{m \cdot \sigma_\eta}{2} \tag{4}$$

The material starts to crack when $\bar{\sigma}_1$ equals to the uniaxial macroscopic tensile strength f_t. Note that the tensile strength of the

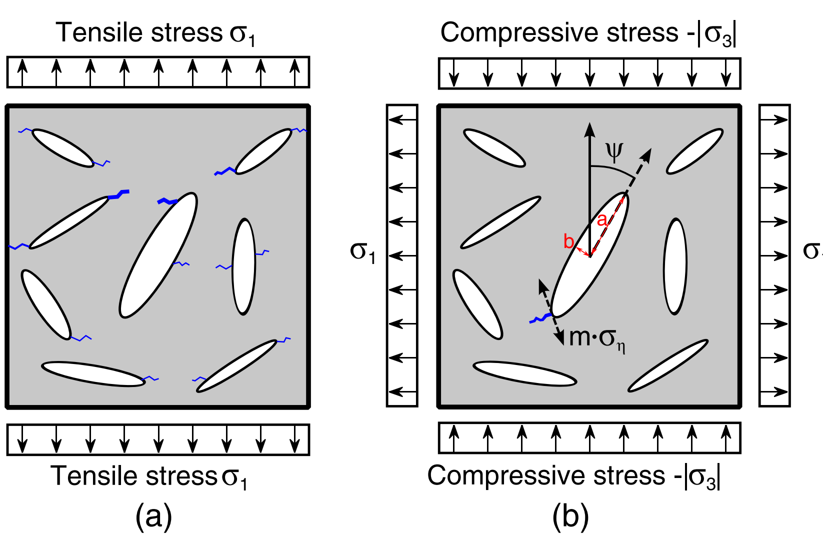

Fig. 1. Crack evolution during (a) uniaxial tensile stress and (b) compressive stresses. The material contains randomly oriented elliptical voids with negligible area.