X International Conference on Computational Plasticity
COMPLAS X
E. Oñate and D.R.J. Owen (Eds)

ON A MICRO-MESO TWO-SCALE DAMAGE MODEL FOR CONCRETE

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Key words: Concrete, Microstructural damage, Multiscale model

Summary. In this contribution, we present the mechanical behaviour of the hardening cement paste explicitly taking into account its complex microstructure. The microstructure of the cement paste is obtained via numerical cement hydration simulation. A simple nonlocal isotropic damage model is adopted for different constituents of the cement paste. The information computed at this microscale is transfered to the matrix phase of the matrix-aggregate-ITZ mesoscale model through a domain decomposition method.

1 INTRODUCTION

In this paper, we present preliminary results of the mechanical behavior of the hardening cement paste (CP). The cement paste, at micro level, is composed of unhydrated cement particles, hydration products and capillary pores. It is the topology of this microstructure of the CP that controls the behaviour of concrete at mesoscale and macroscale. We have used a cement hydration model [2] to create the microstructure of the cement paste. This microstructure is then discretized into finite elements where a simple nonlocal damage constitutive law is applied to each microstructural constituent. The microscale result will be used in a mesoscale model thereby forming a micro-meso two-scale damage model for concrete. Since our work employs purely computational techniques, it complements experimental mechanics particularly at the microscale since it is difficult or even impossible to do experiments on concrete samples at this very small scale (typically about 100 μm). In the present paper, we focus on the microscale analysis and a possible upscaling strategy to bring microscale information up to the mesoscale is announced.

The procedure is such that a three-dimensional representation of the CP is obtained through cement hydration simulations of which a slice is input to a mesh generation code that produces a mesh which will be used for mechanical tests.

2 NUMERICAL CEMENT HYDRATION MODEL

To simulate the microstructure of the cement paste, we have used the cement hydration model of [1] and implemented it in a flexible manner following the work described in [2][1]. Although the implemented model is, in principle, able to model any particulate chemical reactions, in this presentation only the reaction of tricalcium silicate (C_3S) with water producing silicate hydrates (CSH) and Portlandite (CH) is considered.

3 FINITE ELEMENT MODEL

3.1 Finite element discretization

To mesh the microstructure of the cement paste we have used the meshing module of the OOF program [2]. The input of OOF's mesher is a digital image which can easily be obtained from the cement hydration program. Figure 2 shows an example of using OOF's mesher to obtain the unstructured mesh of a slice of a three-dimensional CP.

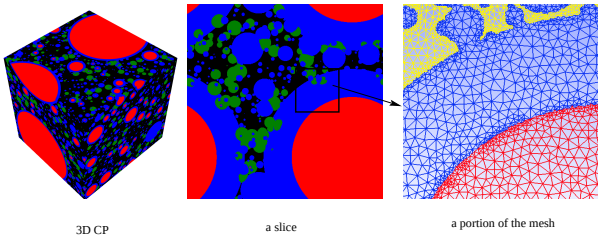


Figure 1: Meshing the microstructure of cement paste.

3.2 Constitutive models

In order to simulate the tensile damage of the CP, we have employed the simple isotropic damage model regularized by the gradient enhanced method [3]. Damage is governed by an exponential law and the damage driving force is chosen to be of Mazars definition, respectively

$$\begin{aligned} \omega &= 1 - \frac{\kappa}{\kappa_I}[1 - \alpha + \alpha \exp^{-\beta(\kappa-\kappa_I)}] \quad \kappa \geq \kappa_I \\ \omega_{\text{eq}} &= \sqrt{\langle\epsilon_1\rangle^2 + \langle\epsilon_2\rangle^2 + \langle\epsilon_3\rangle^2} \end{aligned} \tag{1}$$

where α (residual stress), β (softening slope) and κ_I (damage threshold) denote inelastic parameters and ϵ_i represents the principal strain. The values of the various material parameters are tabulated in Table 1. The Young's moduli and Poisson ratios, which are normally obtained through nano-indentation methods, are taken from [5] whereas the inelastic parameters have been chosen without any experimental base [3].

[1] The only assumption we have made is the spherical shape for cement particles. The major advantage of this vectorial model is the ability to model particles of any size.

[2] For details, see http://www.ctcms.nist.gov/oof

[3] Currently, no experiment has been conducted on specimens of micro size

	Unhydrated	Hydrates	Pore
$E[N/mm^2]$	132700	24000	1.0
ν	0.3	0.24	0.0
κ_I	-	5e-06	-
α	-	0.95	-
β	-	1500	-

Table 1: Material parameters of different phases

4 NUMERICAL RESULTS

In this section, we present some results of a hardening CP specimen of a $200 \times 200 \times 200$ μm^3 unit cell containing 886383 cement particles whose diameters range from 0.5 μm to 40 μm. The water to cement ratio is 0.4. This CP was hydrated for a period of 8 simulated years. Figure 2a shows a partial mesh of a slice through the center of the specimen. [4] The red color denotes unhydrated material, the blue color for the hydration products and the yellow color represents the pores [5]. Figure 2b is the mesh as in 2a but now the pores are not meshed[6].

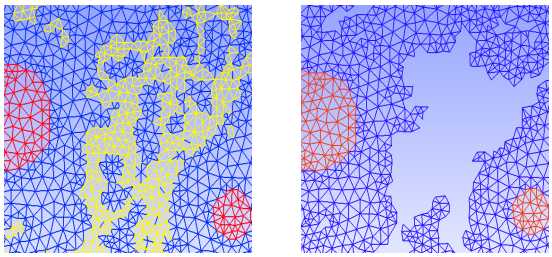


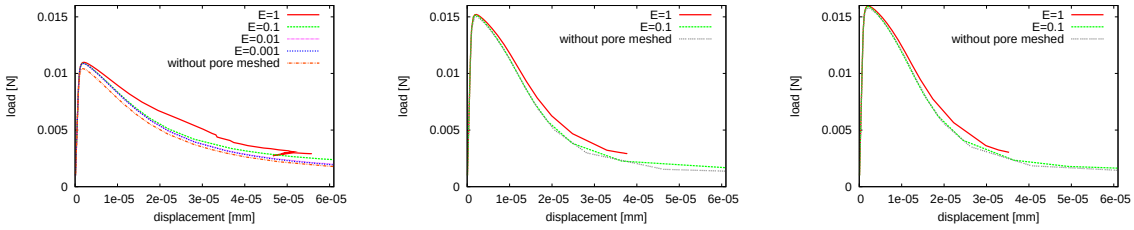
Figure 2: FE discretizations of a slice of a CP specimen: with and without meshing pores.

We have performed tests on two meshes, one with the pores given weak Young's moduli and another one where the pores are not meshed. In Figure 3, the result of uniaxial tensition test is shown where α_d, f_p are the degree of hydration and the pore fraction, respectively. In reducing the Young's modulus of the pores, the load-displacement curves converge to the one obtained without meshing the pores. For specimens which are more hydrated, see Figure 3b-c, even a small reduction in Young's modulus led to the response obtained without meshing the pores. This is expected since more hydrated material means less pores.

[4] We had to limit our FE calculations to two dimensions mainly due to limited computer resources.

[5] We had to mesh the pores since without doing so, due to the presence of solid phases not connecting to the surrounding the stiffness matrix is singular

[6] To produce this mesh, we employed an algorithm which is a simple instance of the fast marching method to remove not only pore elements but also isolated elements



(a) 28 days, α_d=0.86, f_p=11.54% (b) 243 days,α_d=0.97, f_p=5.47% (c) 730 days,α_d=0.99, f_p=4.38%

Figure 3: Comparison between pore and meshed pores with varying Young's moduli.

5 CONCLUSIONS

We presented a numerical tool for damage analysis of concrete specimens at microscale. The numerical tests showed that the pores should not be discretized. In an other case, the Young's modulus of the pores must be chosen carefully. The next logical step is to devise a method to upscale this microscale model of CP to the matrix phase of the mesoscale model [7].

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[7] One potential strategy is the domain decomposition method where the domain is partitioned in such a way that the aggregates, the ITZ and the matrix belong to three distinct partitions. The microscale CP will be projected to the matrix partitions.