Concrete Material – numerical simulation of concrete matrix

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ABSTRACT

Engineering properties of concrete material used in structural analysis and design are commonly based on empirical work. Scientific insight into the mechanical behaviour of the concrete can be gained by studying its microstructure and interaction of its constituents through numerically simulated computational models. The paper presents a methodology of numerical simulation of the concrete material and results of numerical experiments. A hierarchic modeling approach is adopted to obviate numerical problems associated with large difference in the length scales of the constituents. The concrete is considered as a matrix of cement mortar and coarse aggregates, the mortar as a matrix of cement paste and fine aggregates and the cement paste as a porous material. Results of numerical experiments on simulated 2-D test specimens under uniaxial compression load demonstrate that the methodology is capable of capturing characteristic constitutive behaviour and cracking patterns of concrete material. After appropriate validations, it could serve as a numerical laboratory to study different aspects of concrete material behaviour.

INTRODUCTION

Macro behaviour of concrete is a result of complex interaction of its constituents at micro level. It is imperative to understand microstructure and study micro-mechanical properties of concrete material to gain scientific insight into its behaviour. Concrete is broadly considered as a three-phase material consisting of porous cement paste (CP), aggregates and a microsize region of CP around aggregate boundaries called inter-facial transition zone (ITZ). The CP is a composite matrix of unhydrated cores of cement particles, different hydration products like silicate hydrates and calcium hydroxide, and pores of different sizes known as capillary pores. The hydrates of various compounds are collectively referred to as gel. The gel itself has interstitial voids called gel pores that are an order or two finer than the capillary pores [1]. Mechanical properties of hardened CP are largely governed by physical structure of the products of hydration and the physical structure is controlled by the particle size distribution and chemical composition of the cement, the water/cement ratio and the reaction temperature. The aggregates usually consist of two fractions, fine and coarse, collectively occupying about 50-70% of the concrete volume. The fraction having size less than about 5 mm constitute the fine aggregates (FA) and the remaining fraction is the coarse aggregates (CA). The CA occupies about 35-50% of the total volume of concrete. The maximum size of coarse aggregates range from 10 to 40 mm and the most commonly used maximum size is 20-25 mm.

Mechanical properties of the aggregates that affect concrete behaviour significantly are compressive strength and modulus of elasticity. A large variation exists in these properties because of the variation inherent in natural rocks from which these aggregates are manufactured. Other significant aggregate properties that affect the concrete behaviour are particle shape and size, grading, surface texture and water absorption [2]. The CP in the ITZ has higher porosity and inferior mechanical properties due to constrained packing of the cement particles. The ITZ affects the concrete behaviour substantially with respect to strength and cracking.

Empirical modeling work has been the most common tool to study engineering properties of all cement-based materials. The physical sample testing approach employed for the empirical work has many limitations with regard to size, boundary conditions, large variation in the properties of individual constituents and their effects besides the factors like time, cost, efforts and resources. Extensive use of computational techniques have been made in recent times for materials science research such as simulation of microstructure based models of composite materials as well as atomistic/molecular models of pure materials to derive their constitutive behaviour. The complexities of the microstructure of cement-based materials make them perhaps the best candidates for scientific study of the material behaviour such as stress-strain, cracking, fracture, shrinkage and ageing degradation through computational methods.

The objective of the paper is to present a methodology of numerical simulation of concrete material, particularly the cement paste and the mortar/concrete matrix, and results of studies conducted on the simulated models with regard to stress-strain and cracking behaviour of these materials. It is expected that the methodology, after further refinement, could serve the purpose of a numerical concrete laboratory to study different aspects of concrete material behaviour.

NUMERICAL SIMULATION METHODOLOGY

It is currently impractical to develop a unified computational model of concrete incorporating all its constituents because of the range of length scales involved in representing their microstructures. Therefore a hierarchic modeling
approach is adopted. It is apparent to include all the three phases of concrete material in computational models meant to study its micro-mechanical behaviour. However the current work does not include model for the ITZ. The concrete is modeled as a two phase material consisting of the CA and cement mortar. Constitutive input for the mortar phase in the concrete model is derived from another model that simulates the mortar again as a matrix of the FA embedded in the CP. The aggregate is considered as a linear, elastic material and its material properties may be derived from the parent rock properties. The CP is simulated as a porous medium. This model of the CP provides constitutive relation for the paste that goes as an input for the mortar model. The solid portion of the paste is assumed to behave like a rock material. Numerical simulations similar to the model described above for concrete were reported with two phases taken either as aggregates and mortar [3] or aggregates and cement matrix [4]. Triangular elements were used in both these simulations for finite element (FE) discretization and constitutive formulations specific to the problem under study were adopted. FE discretization becomes rather simple when triangular elements are used. In the current work FE discretization is done completely with quadrilateral elements because of the computational advantages. Another important feature of the current approach is the flexibility it offers with respect to the development of constitutive formulations for varied microstructures, varied properties of the constituents and applicability to varied field problems. This makes the current approach versatile enough to put to different numerical experiments on composite materials. The entire methodology of simulating the topology and the FE discretization has been automated into a program ‘COMAT’ (COmposite MATerial) developed by the author which require only the basic design parameters like the water-cement ratio, the pore size, the aggregate fraction and the maximum size of the CA as inputs.

Concrete and Mortar Matrix

A concrete/mortar matrix topology is developed on the basis of volume fraction of aggregates that turns out to be the area fraction in 2-D plane stress condition assumed in the current work. It is possible to generate the topology for different characteristic size (derived from the maximum size and grading of aggregates) as well as different volume fraction of aggregates. For any given characteristic size and volume fraction of aggregates, it is possible to have different random distributions of aggregates in the matrix. The space between the aggregates represents the mortar (incase of concrete matrix) or the cement paste (in case of mortar matrix). The topology is then discretized into finite elements. To generate the topology, randomly distributed points are defined first in the given region. Number of such points is calculated from the volume fraction and the characteristic size of the aggregates, each point representing an aggregate pole. Then the region is sub-divided into voronoi polygons centered around each of the predefined points [5]. Aggregate kernels are obtained by shrinking these polygons around their poles to obtain desired volume fraction of the aggregates. Typical topologies of a concrete matrix and a mortar matrix are shown in figures-1 (a) and (b) respectively.

![Concrete Matrix](image1.png)  ![Mortar Matrix](image2.png)

Fig.1 Numerically Simulated Topologies of Concrete & Mortar Matrices

The aggregate kernels are discretized first followed by the space between them in such a way that well shaped quadrilaterals are obtained. FE discretization of the topology of concrete matrix depicted in figure-1 (a) is shown in figure-2.
Cement Paste Microstructure

In the current work, the CP is assumed as a porous material comprising of solid fraction and voids fraction. The voids fraction, representing the capillary pores, is calculated from the water-cement ratio and the characteristic size of the capillary pores. Two typical simulated topologies of the CP microstructure are shown in figures-3 (a) and (b) in which the voids fraction and the characteristic pore size are kept same in both cases while the random distribution of the pores is different.

This is rather a simple representation of the paste microstructure. It is possible to refine it further by considering the solid fraction also as a porous material consisting of solid gel fraction and gel pores. This is however not incorporated in the current work. It may be noted that the actual microstructure of the CP, as described in the introduction, is very complex and it is currently a challenge to simulate it realistically. Therefore a simplified approach have been adopted that can be validated through physical experiments. It may also be mentioned here that the ITZ is also an inferior form of the CP and thus its simulation can be attempted on similar lines.
RESULTS OF NUMERICAL EXPERIMENTS

All numerical experiments reported in this work pertain to uniaxial loading of square specimens under plane stress condition. A layer of rigid loading platens is introduced at top and bottom. Continuity is assumed at platen-specimen interface. This implies that the platens provide restraint against lateral movement of the test material at the interface.

Cement Paste Specimen under Uniaxial Load

An important hypothesis made in this study for the CP under uniaxial loading is that the material fails on attaining a limiting value of principal tensile strain. Arbitrary elastic properties (elastic modulus ‘E’ and poisson’s ratio) are assigned to the solid fraction of the paste and piece-wise linear analysis is performed. Elements attaining the limiting value of the principal tensile strain are assigned a very low E-value and analysis is repeated with the same load. Solution corresponding to a load step is considered as converged when no element crosses the limiting strain. The load is then incremented and the above process is repeated. The load at which no convergence occurs is considered as the peak load. Here onwards the load is reduced in steps, on occurrence of a sharp rise in strain rate of the whole specimen. Two specimens of the CP, as shown in figures 3 (a) and (b), were analyzed. The stress-strain curves under uniaxial compression load for both these specimens are plotted together in figure-4. The cracking patterns of the specimen-1 at peak load and at failure load are depicted in figure-5 while that for the specimen-2 are shown in figure-6.

![Stress-Strain Curves for Cement Paste Specimens under Uniaxial Compression Load](image1)

![Cracking Patterns of Cement Paste Specimen-1 under Uniaxial Compression Load](image2)
Two non-linear analyses were performed on the mortar specimen of figure-1 (b) under uniaxial compressive load with two different constitutive inputs for the CP fraction (figure-4) while keeping the elastic properties of the FA (E-value in the order of 10^6 MPa and Poisson’s ratio of 0.01) same in both cases. The stress-strain curves obtained from the two analyses are plotted together in figure-7 whereas the cracking patterns at an intermediate load as well as at peak load are shown in figures-8 (a) and (b) respectively. The cracking patterns from both the analyses are identical and thus only one set is presented.
Concrete specimen under Uniaxial Load

Two non-linear analyses were performed on the concrete specimen of figure-1 (a) under uniaxial compressive load with two different constitutive inputs for the mortar fraction (figure-7) while keeping the elastic properties of the CA same as that of the FA in both cases. The stress-strain curves corresponding to the two analyses are shown in figure-9 and the cracking patterns at an intermediate load as well as at peak load are shown in figures-10 (a) and (b) respectively. The cracking patterns for both the analyses are identical and thus only one set is presented.
DISCUSSION OF RESULTS

It is important to note that the numerical experimentation results presented in previous paragraphs correspond to arbitrary choice of the test specimens and the constitutive properties of the basic material phases. The objective is to demonstrate the methodology of numerical simulation of concrete material and its potential. Therefore these results should be viewed in a qualitative sense with respect to the capability of the numerical models to capture the characteristics of the constitutive behaviour and failure pattern of the concrete material rather than quantitative description that would require extensive calibration of the models and the methodology against physical experimental results. As regards the stress-strain curves, it was possible to derive post-peak curve for the cement paste due to the methodology of analysis adopted for this material while is was not possible incase of mortar/concrete due to the software/element limitations of the non-linear analysis adopted for these materials.

The author witnessed large number of uniaxial compression tests on cubes made of the cement paste, the mortar and the concrete at concrete technology laboratories of some important projects in India (see acknowledgement). The shapes of stress-strain curves as well as the cracking patterns of these materials, as obtained from the numerical experiments presented here, have very high similarity with the experimental results. As expected, the stress-strain curve of the cement paste show very little non-linearity near the peak and the cracking/failure of the cement paste specimens does not show any discernible pattern like inclined shear bands or vertical cracks typical of the mortar/concrete specimens. The difference in the stress-strain curve (figure-4), the peak load (figure-4) and the cracking pattern (figures-5 and 6) of the two cement paste specimens, with same pore volume fraction and characteristic pore size but different distribution of pores, indicate the inherent randomness in the constitutive behaviour of this material. The impact of this behaviour is also seen in the mortar/concrete constitutive behaviour but the cracking pattern of these materials is unaffected. This indicates that though the peak load and stress-strain curves of mortar/concrete are affected by cement paste constitution but cracking/failure pattern of these materials is governed by distribution/grading of the aggregates and not much effect of the cement paste is seen.

The stress-strain curves of both the mortar and the concrete show non-linearity at very early load as also seen in the physical tests. The cracking/failure pattern of the mortar/concrete specimens obtained from the numerical experiments with full frictional constraint of the loading platens show striking similarity to the physical experiments. In these materials, the cracks originate near the aggregate boundaries and the failure band is formed at peak load by coalescence and localization of these cracks. This is evident from the numerical experimentation results shown in figures-8 & 10. It may be noted that the initiation of cracks does occur near the aggregate boundaries inspite of absence of the interfacial transition zone in the current
The reason for this can be found in the difference in the elastic properties of the two interfacing materials causing stress concentrations.

CONCLUDING REMARKS

A methodology of numerical simulation of cement-based materials is presented. Results of preliminary numerical experiments are promising towards further pursuance of the methodology. The hypothesis of failure of the cement paste based on limiting principal strain seems to be in the right direction. However this would require further calibration/validation.

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REFERENCES