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Numerical simulation of plain concrete specimens with micromechanical model and simple lattice model

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In this paper, a recently proposed micromechanical model for concrete is combined with a simple lattice model to simulate the behaviours of plain concrete specimens under tension, compression and three-point bending. The Mori-Tanaka method based micromechanical model for concrete considers the microcracks around the mortar-coarse aggregate interface and the aligned coalesced cracks in the concrete. It explicitly correlates the mechanical properties of concrete with the properties of its constituents such as mortar and coarse aggregates. The adopted simple lattice model, in which the axial interaction between neighbouring points is considered as a truss, does not need to generate grain structure and is thus easy to implement. Hence, this combination can be used to investigate the influences of the concrete constituents' properties on the behaviours of the concrete specimens in a simple way. The predicted deformation responses and crack patterns from the computational model are generally in agreement with the experimental observations.

Notation

A	cross-sectional area of truss element
c_0, c_1	volume fractions of mortar and coarse aggregate
c_i	fraction of failed interfaces
c_v	volume ratio of aligned cracks to overall concrete
E_0, E_1	initial elastic moduli of mortar and coarse aggregate
E_e	Young's modulus of concrete with imperfect interfaces
E_{xx}	stiffness of truss element
f'_c	compressive strength of concrete
g	diameter of coarse aggregates
I	identity matrix
K^e	secant stiffness matrix of truss element
L	final secant material matrix of concrete
L_e	material matrix of concrete with imperfect interface
l	length of truss element
m_2	shape factor in volume ratio of aligned cracks to overall concrete
S	Eshelby's tensor
w	density of concrete
α_F	coefficient
ε	effective strain of concrete
ε_1	first principal tensile strain of concrete
ε_{u2}	ultimate tensile strain value
κ_0, κ_1	bulk moduli of mortar and coarse aggregate

κ_d, κ_p	bulk moduli of concrete with destroyed and perfect interface
κ_e	equivalent bulk modulus of concrete
μ_0, μ_1	shear moduli of mortar and coarse aggregate
μ_d, μ_p	shear moduli of concrete with destroyed and perfect interface
μ_e	equivalent shear modulus of concrete
ρ_0, ρ_1	densities of the mortar and coarse aggregate
σ	stress vector of concrete
ν_0, ν_1	Poisson ratios of mortar matrix and coarse aggregate
ν_e	Poisson ratio of concrete with imperfect interfaces

Introduction

A lot of research works, driven by the development of powerful computers, have simulated the failure or fracture behaviours of concrete specimens. The traditional methods employ the finite-element method (FEM) combined with certain constitutive models, such as discrete cracking models, smear cracking models, as well as damage models (ACI, 1997). However, in these macroscopic constitutive models, the model parameters and constants are usually empirical parameters and they do not reflect the real material properties of the concrete and its constituents, namely, mortar and coarse aggregates. Hence, these traditional methods could not be used to investigate

the influences of the concrete constituents' properties on the behaviours of the concrete specimens.

On the other hand, some discrete models or lattice models for concrete were developed to model the concrete specimen as a system of discrete elements such as particles, trusses, or frames. This type of model does not model the material continuously, but replaces the continuum by an array of discrete elements in the form of particles in contact, trusses, or frames, in such a manner that the displacements are defined only at the centres of the particles, or at the nodes of the truss or frame.

The beginning of the particle approach can be traced back to the development of the distinct element method by Cundall (1971), Serrano and Rodriguez-Ortiz (1973), Kawai (1980) and Cundall and Strack (1979), in which the behaviour of material was analysed by the interactions of the particles in contact. Later the method of the particle model was extended further to simulate the behaviour of brittle composite materials, especially for concrete (Arslan *et al.*, 2002; Bolander and Saito, 1998; Cusatis *et al.*, 2003, 2011; Mohamed and Hansen, 1999; Zubelewicz and Bazant, 1987).

Generally there are two ways to describe the heterogeneity of concrete with a lattice model (Schlangen and van Mier, 1992). The first method is to generate the grain structure of the concrete with a Fuller curve, which is usually chosen as the distribution of the diameters of the intersection circles (or the spherical aggregate particles). Then, a lattice is projected onto the generated grain structure, and different strengths and stiffnesses are assigned to the respective bar elements; in other words, when a bar element is situated inside an aggregate particle, the stiffness and the failure strength of the aggregate will be assigned to this element; a bar element located on the boundary between aggregate and mortar will be considered as the interface; and mortar properties will be assigned to those bar elements projected on the mortar matrix. As the heterogeneity of the concrete has been introduced in a realistic way, this method is widely used to simulate the behaviours and fracture properties of concrete (Elias and Stang, 2012; He *et al.*, 2012; Kozicki and Tejchman, 2007; Zheng *et al.*, 2011).

The second method needs not generate the grain structure, and this is simply to specify a statistical distribution of material property, that is, the tensile strength of concrete to bar elements in the lattice. This method is much easier to implement. However, in this method the effects of the concrete's constituents are not explicitly included. Hence, unlike the first method, it cannot reflect the influences of the concrete constituents' properties on the behaviours of the concrete specimens. In this paper, a simple lattice model without the grain structure is used to simulate the behaviour of concrete, together with a recently proposed micromechanical model (Teng *et al.*, 2014). As the material properties of concrete, obtained from the micromechanical model, are determined by the properties

of the concrete constituents, namely, the elastic moduli, Poisson ratios and volume ratio of mortar and coarse aggregates, it is possible to investigate the influences of the concrete constituents' properties on the behaviours of the concrete specimens, using the simple lattice system and the recently proposed micromechanical model.

In this paper, the axial interaction between neighbouring points is considered as a truss. The initial moduli of truss members are the initial elastic modulus of concrete. With the increase of loading, the moduli of the truss members will decrease. As shown in Figure 1, there are two types of truss failure. The typical compressive and tensile stress–strain curves are shown in Figure 2 and Figure 3, respectively. A recently proposed micromechanical model for concrete under static load (Teng *et al.*, 2014) is used as the basic constitutive relations of concrete, and this works together with a simple lattice model to predict the behaviour of concrete specimens under uniaxial tension, compression and three-point bending.

Micromechanical model for concrete

In the recently proposed micromechanical model for concrete (Teng *et al.*, 2014), the concrete is considered as a two-phase composite (mortar + coarse aggregates). Two kinds of defects are considered, namely, microcracks around the mortar–coarse aggregate interface or the interfacial transition zone (ITZ) and aligned coalesced cracks in the concrete. First, a two-phase composite (mortar + spherical coarse aggregates) is considered. The degradation of the mortar–coarse aggregate interfaces is modelled as the progressive failure of the spring layers. Under the frame of the Mori–Tanaka method, the bulk and shear

Figure 1. Failure model of truss

Figure 2. Typical uniaxial compression

Figure 3. Typical uniaxial tension

moduli of concrete with destroyed interfaces, κ_d and μ_d , are

$$1a. \quad \kappa_d = \kappa_0 + \frac{(2/3)c_1\kappa_0(\kappa_1 - \kappa_0)}{\kappa_0 + (c_1/3 + c_0)(\kappa_1 - \kappa_0)}$$

$$1b. \quad \mu_d = \mu_0$$

where the volume ratios of mortar (c_0) and coarse aggregate (c_1), and their bulk and shear moduli (κ_0 , μ_0 , κ_1 and μ_1) are given properties of concrete constituents, and they can be calculated from their densities (ρ_0 , ρ_1), initial elastic moduli (E_0 and E_1) and Poisson ratios (ν_0 and ν_1), that is (Teng *et al.*, 2014)

$$1c. \quad c_0 = \frac{w - \rho_1}{\rho_0 - \rho_1}, \quad c_1 = 1 - c_0$$

$$1d. \quad \kappa_0 = \frac{E_0}{3(1 - 2\nu_0)}, \quad \mu_0 = \frac{E_0}{2(1 + \nu_0)}$$

$$1e. \quad \kappa_1 = \frac{E_1}{3(1 - 2\nu_1)}, \quad \mu_1 = \frac{E_1}{2(1 + \nu_1)}$$

where w is the density of concrete. Similarly, the bulk and shear moduli of concrete with perfect interfaces, κ_p and μ_p , are

$$2a. \quad \kappa_p = \kappa_0 + \frac{3(1 - \nu_0)c_1\kappa_0(\kappa_1 - \kappa_0)}{3(1 - \nu_0)\kappa_0 + c_0(1 + \nu_0)(\kappa_1 - \kappa_0)}$$

$$2b. \quad \mu_p = \mu_0 + \frac{15(1 - \nu_0)c_1\mu_0(\mu_1 - \mu_0)}{15(1 - \nu_0)\mu_0 + 2(4 - 5\nu_0)c_0(\mu_1 - \mu_0)}$$

Hence, the equivalent bulk and shear moduli of concrete with the fraction of failed interfaces c_i are

$$3a. \quad \kappa_e = c_i\kappa_d + (1 - c_i)\kappa_p$$

$$3b. \quad \mu_e = c_i\mu_d + (1 - c_i)\mu_p$$

If κ_e and μ_e are known, the equivalent Young's modulus E_e and the Poisson ratio ν_e of the concrete with imperfect interfaces are

$$4a. \quad E_e = \frac{9\kappa_e\mu_e}{3\kappa_e + \mu_e}$$

$$4b. \quad \nu_e = \frac{3\kappa_e - 2\mu_e}{6\kappa_e + 2\mu_e}$$

In Equation 3, the fraction of failed interfaces c_i is calculated as

$$5. \quad c_i(\varepsilon) = \frac{1}{1 - e^{-1}} \left\{ 1 - \exp \left[- \left(\frac{\varepsilon}{0.008} \right)^3 \right] \right\}$$

where ε is the effective strain of concrete; in other words, in the case of uniaxial compression, ε represents the compressive strain.

With further increase of load, the microcracks in the mortar-coarse aggregate ITZ will propagate into the mortar and aggregates and coalesce to cause the failure. These coalesced cracks are considered as a series of aligned cracks perpendicular to the direction of the principal tension strain and they are considered as voids, a kind of material whose moduli are zeros. The final secant material matrix of concrete can be solved, using the Mori-Tanaka method, as

$$6. \quad \mathbf{L} = \mathbf{L}_e - c_v \mathbf{L}_e \mathbf{T} [(1 - c_v) \mathbf{I} + c_v \mathbf{T}]^{-1}$$

with

$$7a. \quad \mathbf{T} = [(1 - c_v)(\mathbf{I} - \mathbf{S})]^{-1}$$

$$7b. \quad \mathbf{S} = \begin{bmatrix} 0 & 0 & 0 \\ \frac{v_e}{2(1 - v_e)} & \frac{5 - 4v_e}{8(1 - v_e)} & 0 \\ 0 & 0 & 1/2 \end{bmatrix}$$

$$7c. \quad \mathbf{L}_e = E_c \begin{bmatrix} \frac{1}{1 - v_e^2} & \frac{v_e}{1 - v_e^2} & 0 \\ \frac{v_e}{1 - v_e^2} & \frac{1}{1 - v_e^2} & 0 \\ 0 & 0 & \frac{1}{2(1 + v_e)} \end{bmatrix}$$

where $\mathbf{I}$ is the identity matrix; $\mathbf{S}$ is the Eshelby's tensor; $\mathbf{L}_e$ is the material matrix of concrete with imperfect interface, which is obtained from Equation 4; and c_v is the volume ratio of aligned cracks to overall concrete volume, that is

$$8. \quad c_v(\varepsilon_1) = \frac{1}{1 - e^{-1}} \left\{ 1 - \exp \left[- \left(\frac{\varepsilon_1}{\varepsilon_{u2}} \right)^{m_2} \right] \right\}$$

where ε_1 is the first principal tensile strain of concrete; ε_{u2} is the ultimate tensile strain value (when ε_1 reaches the value of ε_{u2} , the concrete fails completely); and m_2 is the shape index. The ultimate tensile strain value ε_{u2} is related to the diameter of the aggregates (g) and the compressive strength (f'_c), that is

$$9. \quad \varepsilon_{u2} = 2.5143 f'_c{}^{0.2} \frac{\alpha_F}{g}$$

where the coefficient α_F can be 4, 6 or 10 when the diameters of aggregates, g , are 8 mm, 16 mm or 32 mm, respectively. A suitable value of m_2 was found to be

$$10. \quad m_2 = 8.4 - 7.55 \exp(-0.1 \rho^{3.57})$$

where

$$\rho = \frac{\varepsilon_{u2}}{[3.34 - 1.59 \exp(-3.1 \times 10^5 \varepsilon_{u2}^{-20.48})]}$$

Given the properties of its constituents, the above micromechanical model is capable of predicting the entire response of mortar and concrete under uniaxial tension/compression and biaxial load (Li, 2001; Teng *et al.*, 2014). It explicitly correlates the mechanical properties of concrete with those of its constituents. Hence, together with a simple lattice model, it can be used to investigate the influences of the concrete constituents' properties on the behaviours of the concrete specimens.

Formulation of element stiffness matrix

In the above micromechanical model, the current moduli of concrete are calculated based on the current total strain, so it can be directly used with the secant method. Inside the truss element, the concrete is allowed to have the lateral strain as a two-dimensional problem with the only axial-directional force. Its stress-strain relationship can be written, in the local coordinate system, as

$$11. \quad \begin{Bmatrix} \sigma_x \\ \sigma_y \\ \sigma_{xy} \end{Bmatrix} = \begin{bmatrix} L_{11} & L_{12} & L_{13} \\ L_{21} & L_{22} & L_{23} \\ L_{31} & L_{32} & L_{33} \end{bmatrix} \begin{Bmatrix} \varepsilon_x \\ \varepsilon_y \\ \varepsilon_{xy} \end{Bmatrix}$$

where the material matrix $\mathbf{L}$ of concrete is obtained from Equation 6. In Equation 11, the axial strain ε_x can be obtained from the nodal displacements and the stress components σ_y and σ_{xy} are zeros, as the truss element is under axial load. Hence, the axial stress-strain relationship can be condensed as

$$12a. \quad \sigma_x = \left(L_{11} - [L_{12} \ L_{13}] \begin{bmatrix} L_{22} & L_{23} \\ L_{32} & L_{33} \end{bmatrix}^{-1} \begin{bmatrix} L_{21} \\ L_{31} \end{bmatrix} \right) \varepsilon_x$$

or

$$12b. \quad \sigma_x = E_{xx} \varepsilon_x$$

Now the secant stiffness matrix of the truss element is thus

$$13. \quad \mathbf{K}^e = E_{xx} \frac{A}{l} \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}$$

in which the ratio of the cross-sectional area A to the element length l is considered as a constant, $\sqrt{3}/2$, according to the research works of Hrennikoff (1941) and Mohamed (1997).

Figure 4. Single-edge notch specimen for mortar (Maji and Shah, 1988)

Figure 5. Mesh layout for single-edge notch specimen

Implementation of models

In this paper, the PDE toolbox of Matlab is employed to create a regular triangle mesh, and then the nodes and the truss elements are translated. If there are some notches in the specimens, more elements will be given in the zones of near notches and Femlab is used to create the mesh.

The developed computer program employs a non-linear finite-element incremental displacement scheme with an iterative procedure based on the successive approximations method (Owen and Hinton, 1980). The program starts by identifying the geometry of the specimens, namely, the coordinate for each of the elements and mesh layout from the data files, which is created by the PDE toolbox of Matlab. Then, the incremental procedure starts and the nodal displacements are solved out. Subsequently, the strain in each element is calculated and checked with the current element status. If the element status has changed in this iteration according to Equations 5 and 8, the new stiffness is assigned to the element based on the updated status. After updating the status of all elements, the overall stiffness is recalculated. If the ratio of the norm of the displacement vector in the current iteration to that in the last iteration satisfies the prescribed tolerance, the current increment is considered as convergent and the required information for the current increment is recorded. Otherwise the iteration procedure is continued. When the volume ratio of aligned cracks to overall concrete volume c_v is greater than 0.9, the element is considered to have cracked or failed. The computer program is provided with the capability to draw this 'crack'.

Simulation of direct tension specimen

The above numerical model has been applied to simulate the behaviour of a single-edge-notched specimen under direct

tension. At the same time, the process of localisation as well as the development of cracks was studied based on the proposed model. As the first example, a plain mortar specimen under direct tension (Maji and Shah, 1988) is simulated. The geometry for the direct tension specimen is shown in Figure 4. The corresponding mesh layout with 1348 nodes and 3941 elements is shown in Figure 5 and the corresponding material properties

E_0 : GPa (ksi)	f_c : MPa (ksi)	c_0
28.9 (4191)	37.33 (5.41)	1

Table 1. Mortar properties for direct tension simulation

Figure 6. Theoretical and experimental load-CMOD curve for single-edge notch tensile specimen

Figure 7. Crack patterns for single-edge notch tensile specimen at loading points A, B, C and D

Figure 8. Notched beam for three-point bending (Petersson, 1980)

Notch depth: mm (inch)	f_c : MPa (ksi)	E_c : GPa (ksi)	E_0 : GPa (ksi)	E_1 (estimated): GPa (ksi)
25 (1)	53 (7.69)	41 (5946)	36.55 (5301)	50 (7252)

Table 2. Material properties of three-point bending (Petersson, 1980)

Figure 9. Mesh layout for three-point bending

are shown in Table 1. The load–deformation response under splitting tension simulated by the proposed numerical model generally conforms to the experimental result, as shown in Figure 6. At the same time, the crack patterns at four loading points are shown in Figure 7.

Figure 10. Theoretical and experimental curve for three-point bending

Figure 11. Crack pattern at loading points A, B, C and D

Simulation of three-point bending specimen

Bending is a typical loading pattern in concrete structures. Thus many research studies are focused on the field, either theoretically or experimentally. A considerable number of tests of specimens under bending have been conducted. In this paper, a typical example is chosen to compare with the results

Figure 12. Specimen configurations for compression simulation

Figure 13. Mesh layout for compression simulation

f_c : MPa (ksi)	E_c : GPa (ksi)	E_1 : GPa (ksi)	E_0 : GPa (ksi)
30.87 (4.48)	26.28 (3811)	59.6 (8644)	16.944 (2457)

Table 3. Material properties for compression simulation

Figure 14. Predicted stress-strain curve under compression

of numerical simulations using the micromechanical model and the simple lattice model.

Petersson (1980) completed some three-point bending tests on notched beams. Here, a typical three-point bending beam from Petersson's results was used to study the capability of the proposed numerical model to predict the behaviour of plain concrete specimens under three-point bending. The dimensions of specimens are shown in Figure 8 and material properties are given in Table 2, where the elastic modulus for aggregates is assumed.

According to the material properties given in Table 2 and mesh layout shown in Figure 9, the corresponding load-displacement curve from the proposed numerical model again

Figure 15. Crack pattern under compression at loading points A, B, C and D

generally agrees with the experimental result, as shown in Figure 10. At the same time, the corresponding crack patterns at four loading points are shown in Figure 11.

Simulation of uniaxial compression specimen

For concrete, its compressive behaviour is one of its most important properties. Extensive research studies have focused on the compressive behaviour of concrete, either theoretically or experimentally. In this research, the proposed numerical model has also been used to simulate the behaviour of concrete specimens under compression. Here a $200 \times 200 \times 50$ mm specimen from the experiments of Kupfer *et al.* (1969) is chosen for simulation.

The geometry of the specimen is shown in Figure 12 and the corresponding mesh layout is drawn in Figure 13. The material properties are listed in Table 3. The corresponding stress–strain curve is obtained in Figure 14 and the crack patterns at four loading points are shown in Figure 15. In this example, it shows that the model could predict most of the experimentally observed phenomena for concrete under compression, including softening, localisation of deformation and crack patterns. However, the prediction for the deformation at ultimate load generally gives a lower value. The predicted strain at ultimate load is about 0.001, whereas the value from experimental data is around 0.002. Many researchers have pointed out the problems and provided some explanations (Bazant and Planas, 1998; Mohamed, 1997; van Mier, 1997). This is not a drawback in the model, but in the way that the specimens are simulated. Compressive behaviour of concrete is a triaxial phenomenon, and the crack surfaces are usually located in more than one plane. Thus, a three-dimensional simulation is essential for predicting the compressive behaviour; however, the prediction of the current two-dimensional model still could provide valuable information about the response of concrete under compression.

Conclusions

In this paper, a recently proposed micromechanical model for concrete was combined with a simple lattice model to simulate the behaviours of plain concrete specimens under tension, compression and three-point bending. The micromechanical model used for concrete explicitly correlates the mechanical properties of concrete with the properties of its constituents. The simple lattice model employed does not generate grain structure and is thus easy to implement. Hence, this combination can be used to investigate the influences of the concrete constituents' properties on the behaviours of the concrete specimens in a simple way.

The predicted deformation responses and crack patterns from the computational model are found to be generally in agreement with the experimental results. The computational model can, therefore, be an effective and useful tool for the analysis

of microstructure-related behaviours of concrete. Future work may be focused on a three-dimensional simulation to study concrete behaviours related to three-dimensional actions.

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