Modeling Fracture Processes in Numerical Concrete

Zhiwei Qian^{1,2,*}, Erik Schlangen², Guang Ye², Klaas van Breugel²

¹ Materials innovation institute M2i, Delft, the Netherlands
² Delft University of Technology, Delft, the Netherlands
* Corresponding author: z.qian@tudelft.nl

Abstract Modeling the fracture processes in concrete requires a material structure of concrete to start with. The material structure of concrete can be obtained either experimentally by X-ray computed tomography, or numerically by a computer simulation. A simplified way to represent the material structure of concrete is to put multiple spheres in a matrix, where the spheres are interpreted as aggregates. This assumption of the shape of aggregates might have influences on the fracture processes in concrete, such as the microcracks propagation path. Recently the Anm material model was proposed and implemented, which can produce a material structure of concrete with irregular shape aggregates. The irregular shape is represented by a series of spherical harmonic coefficients. The further mechanical performance evaluation would benefit from this more realistic material structure. In this paper a material structure of concrete is simulated by the Anm material model. A number of irregular shape particles are planted in a matrix. This material structure is then converted into a voxelized image. Afterwards a random lattice mesh is made, and three types of lattice elements are defined, which represent aggregates, matrix and interface respectively. A uniaxial tensile test is set up and simulated by fixing all the lattice nodes at the bottom of the specimen and imposing a prescribed unit displacement onto all the nodes at the top. The lattice fracture analysis gives the stress-strain response and microcracks propagation, from which some mechanical properties such as Young's modulus, tensile strength and fracture energy can be predicted.

Keywords Lattice Fracture, Tensile Test Simulation, Irregular Shape Aggregates

1. Introduction

The material structure of concrete determines its global performance. Normal concrete is made from coarse aggregates (e.g. crushed stones, river gravels), fine aggregates (e.g. sands), cement and water. A chemical reaction starts immediately when water is mixed with cement, and reaction products are produced. The resulting cement paste keeps aggregates together and forms a system which is able to carry loads. Mortar consists of cement paste and sand, and concrete is composed of mortar and coarse aggregates.

Generally speaking there are two different approaches to obtain the material structure of concrete, which are X-ray computed tomography and computer simulations. From the modeling point of view, the material structure of concrete can be represented by particles embedded in matrix material model. The particles are interpreted as coarse aggregates, and the matrix as mortar. A simplified way to represent coarse aggregates is to use spheres. However this simplification might alter the real material structure of concrete, and thus may change the fracture processes in concrete, such as the microcracks propagation path. Recently the Anm material model was proposed and implemented, which can produce a material structure of concrete with irregular shape aggregates [1]. The irregular shape is represented by a series of spherical harmonic coefficients. The more realistic material structure would make the prediction of fracture processes more precise.

Numerical modeling of fracture processes in brittle materials, such as cement paste, mortar, concrete and rocks, started in the late 1960s with the landmark papers of Ngo and Scordelis [2] and Rashid [3], in which the discrete and smeared crack models were introduced. Especially the latter approach gained much popularity, and in the 1970s comprehensive efforts were invested in developing constitutive models in a smeared setting which could reproduce the experimentally

observed stress-strain characteristics of concrete. However neither of them could tell the fracture processes in detail. In the 1990s, Schlangen and van Mier proposed another model to compensate the drawbacks of discrete and smeared crack models, which is called lattice fracture model [4].

The concept of lattice was proposed by Hrennikoff in the 1940s to solve elasticity problems using the framework method [5]. In the 1970s and 1980s the lattice model was introduced in theoretical physics to study the fracture behavior of disordered media [6, 7]. In the field of material sciences, a model was proposed by Burt and Dougill to simulate uniaxial extension tests, which consists of a plane pin-jointed random network structure of linear elastic brittle members having a range of different strengths and stiffnesses [8].

In the lattice fracture model, the continuum is replaced by a lattice of beam elements. Subsequently, the microstructure of the material can be mapped onto these beam elements by assigning them different properties, depending on whether the beam element represents a grain or matrix. Various conventional laboratory experiments like uniaxial tensile test, compressive test, shear test, bending test and torsional test can be simulated by the lattice fracture model and the model can be applied towards a wide range of multiphase materials, such as concrete [9], cement paste [10], graphite and fiber reinforced concrete [11].

In this paper a material structure of concrete is simulated by the Anm material model. A number of irregular shape particles are planted in a matrix. This material structure is then converted into a voxelized image. Afterwards a random lattice mesh is made, and three types of lattice elements are defined, which represent aggregates, matrix and interface respectively. A uniaxial tensile test is set up and simulated by fixing all the lattice nodes at the bottom of the specimen and imposing a prescribed unit displacement onto all the nodes at the top. The lattice fracture analysis gives the stress-strain response and microcracks propagation, from which some mechanical properties such as Young's modulus, tensile strength and fracture energy can be predicted.

2. Simulation of the material structure of concrete

The concept of particles embedded in matrix is the essential of the Anm material model. An empty container is created to represent a concrete specimen at the beginning, and then all the particles representing coarse aggregates are placed one after another into this container, from the larger ones to smaller ones. It is good to start with the largest particles as it would be more difficult to place them if they were processed at a later stage. All the particles are separated into several sieve ranges according to the particle sizes indicated by the particle widths. The largest sieve range is processed first, a width within this sieve range is picked randomly and assigned to a particle which is chosen from the appropriate particle shape database. The particle shape database can be created for different classes of aggregates with the procedures proposed in [12]. An arbitrary rotation is performed on the particle to get rid of possible orientation bias, which might be introduced during the production of the particle shape database. After the rotation the particle is placed at a randomly chosen location in the specimen. The particle is checked against all the previously placed particles for overlap. If no overlap is detected, then the particle enters the simulation box successfully, otherwise it will be moved to a new randomly chosen location. The reassignment of the location is subject to a pre-defined maximum number of attempts. After the consecutive failures reach the limit, the particle will be resized to another randomly selected width within the current sieve range, and then be thrown into the specimen following the same trial-and-error procedure. The particle size rescale is also subject to a pre-defined maximum number of attempts. If the rescales do not help, then the particle will be rotated again to have another orientation. If the problem still exits, then a new shape will be chosen from the particle shape database. In case the particle cannot find its

position eventually, it may suggest there is no space available for new particles within the current sieve range. The next sieve range will be processed if no availability for the current sieve range is concluded, or all the particles within the current sieve range have already been placed. The above trial-and-error procedure is called parking procedure and it is the essential of the Anm material model.

Concrete specimen of the size 150 mm in the cubic shape is simulated by the Anm material model. The specimen has two phases, the mortar matrix and crushed stone aggregates. Non-periodic material boundary applies, which requires all the particles are inside the specimen and no part of a particle can pass through a surface. The total mass of the crushed stones is 2653 g, the corresponding volume is 1001132 mm³, and 64% of which are in the sieve 8~16 mm, the rest 36% are in the sieve 4~8 mm. The particle size is taken as the particle width and its distribution for the coarse aggregates is given in Figure 1. The volume percentage of the crushed stones in the concrete specimen is 30%. The simulated material structure of the concrete specimen with irregular shape crushed stones is sketched in Figure 2.

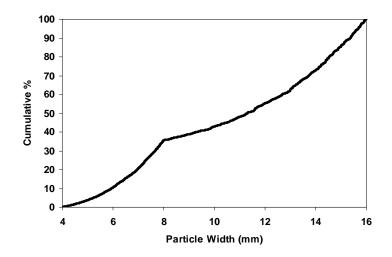


Figure 1. Particle size distribution for the coarse aggregates in concrete

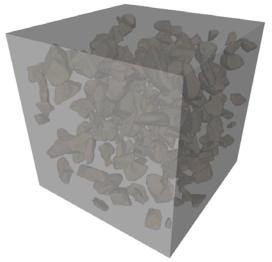


Figure 2. The material structure of the 150 mm concrete specimen with irregular shape crushed stones

3. Fracture processes in the numerical concrete

The fracture processes in concrete can be predicted by the lattice fracture model. The material structure of concrete is obtained in the previous section, and the next step is to evaluate its mechanical performance by simulating a uniaxial tensile test on it. To reduce the computational effect, a smaller specimen of the size 40 mm is cut out from the original 150 mm specimen at its center. The 40 mm concrete specimen is then digitized at the resolution of 1 mm, and consists of two solid phases namely stone and mortar. A lattice network is constructed based on the digital concrete specimen, and three types of lattice elements are identified, which represent crushed stone, mortar and interface respectively, as shown in Figure 3. The local mechanical properties are given in Table 1. The properties of the lattice elements representing mortar are varied randomly to reflect the heterogeneity of mortar phase.

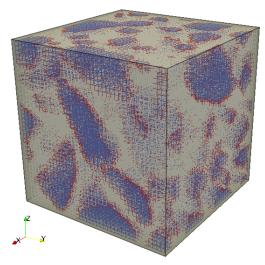


Figure 3. Lattice mesh of the 40 mm numerical concrete specimen

Table 1. Local mechanical properties of stone, mortar and interface elements in concrete				
	Young's modulus (GPa)	Tensile strength (MPa)		
Stone	70	24		
Mortar	17~65	1.1~19.5		
Interface	41	1		

A uniaxial tensile test is simulated on the lattice system meshed from the 40 mm concrete specimen as shown in Figure 3, using the local mechanical properties listed in Table 1. All the lattice nodes on the bottom surface of the specimen are fixed, and a unit prescribed displacement is imposed on the nodes located on the top surface, as illustrated in Figure 4.

The lattice fracture analysis consists of multiple steps. At every analysis step it is required to determine the critical element and the corresponding system scaling factor after the calculation of comparative stress in every lattice element. The critical element is the one with highest stress/strength ratio when the system is loaded by a unit prescribed displacement. The inverse of the ratio is defined as a system scaling factor. The system scaling factor, together with the reactions on the restraint boundaries, determines one scenario of critical load-displacement pairs. The critical element is removed from the system and if the system does not fail completely yet, it is recomputed as the system is updated due to the element removal. Multiple analysis steps are carried out until the system fails. Hence a set of load-displacement pairs can be obtained and used to plot the load-displacement diagram, which can be converted to a stress-strain diagram later to represent the

constitutive relation of the material. The step-by-step removal of critical lattice elements indicates the microcracks evolution in the specimen. Thus the microcracks propagation and the cracks pattern in the final failure state can also be simulated.

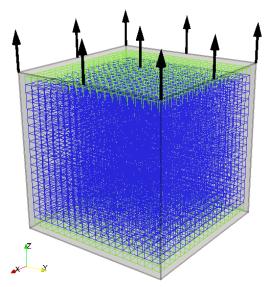


Figure 4. Uniaxial tensile test setup

For the example given in this paper, the resulting stress-strain response is presented in Figure 5, and some mechanical properties can be computed as given in Table 2.

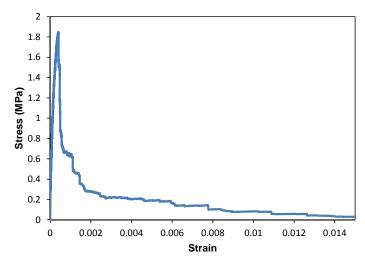


Figure 5. Simulated stress-strain response of the 40 mm concrete specimen

Table 2. Simulated mechanical p	properties of the 40 mm	concrete specimen
---------------------------------	-------------------------	-------------------

Young's modulus (GPa)	Tensile strength (MPa)	Strain at peak load	Fracture energy (J/m ²)
31	1.8	0.04%	127

The pattern of the simulated stress-strain response of the 40 mm concrete specimen is similar to the one observed in laboratory, and the mechanical properties computed from the stress-strain diagram are also located within the reasonable range.

4. Summary and conclusions

In this paper a material structure of concrete is simulated by the Anm material model. A number of irregular shape particles are planted in a matrix, representing coarse aggregates in mortar. This material structure of concrete is then converted into a voxelized image. After that a random lattice mesh is made, and three types of lattice elements are identified, which represent aggregates, matrix and interface respectively. A uniaxial tensile test is set up and simulated by fixing all the lattice nodes at the bottom of the specimen and imposing a prescribed unit displacement onto all the nodes at the top. The lattice fracture analysis gives the stress-strain response and microcracks propagation, from which some mechanical properties such as Young's modulus, tensile strength and fracture energy can be predicted. The simulated mechanical properties of the numerical concrete specimen are quite reasonable, which is a positive evidence that proves the feasibility of the proposed modeling procedures.

Acknowledgements

This research was carried out under project number M83.1.12459 in the framework of the Research Program of the Materials innovation institute M2i (<u>http://www.m2i.nl</u>). Part of this work was sponsored by the European Union FP7 project CODICE (<u>http://www.codice-project.eu</u>).

References

- [1] Qian, Z., Multiscale Modeling of Fracture Processes in Cementitious Materials, PhD thesis, Delft University of Technology, 2012
- [2] Ngo, D. & Scordelis, A., Finite Element Analysis of Reinforced Concrete Beams, J Am Concr Inst, 1967, 64, 152-163
- [3] Rashid, Y., Ultimate strength analysis of prestressed concrete pressure vessels, Nuclear Engineering and Design, 1968, 7, 334-344
- [4] Schlangen, E. & van Mier, J., Experimental and numerical analysis of micromechanisms of fracture of cement-based composites, Cement and Concrete Composites, 1992, 14, 105-118
- [5] Hrennikoff, A., Solution of problems of elasticity by the framework method, Journal of Applied Mechanics, 1941, 8, 169-175
- [6] Ziman, J. M., Models of disorder: the theoretical physics of homogeneously disordered systems, Cambridge University Press, 1979
- [7] Herrmann, H. J.; Hansen, A. & Roux, S., Fracture of disordered, elastic lattices in two dimensions, Phys. Rev. B, American Physical Society, 1989, 39, 637-648
- [8] Burt, N. J. & Dougill, J. W., Progressive Failure in a Model Heterogeneous Medium, Journal of the Engineering Mechanics Division, 1977, 103, 365-376
- [9] Schlangen, E., Experimental and Numerical Analysis of Fracture Processes in Concrete, PhD thesis, Delft University of Technology, 1993
- [10] Qian, Z.; Schlangen, E.; Ye, G. & van Breugel, K., Prediction of Mechanical Properties of Cement Paste at Microscale, Materiales de Construccion, 2010, 60, 7-18
- [11] Schlangen, E. & Qian, Z., 3D modeling of fracture in cement-based materials, Journal of Multiscale Modelling, 2009, 1, 245-261
- [12]Garboczi, E., Three-dimensional mathematical analysis of particle shape using X-ray tomography and spherical harmonics: Application to aggregates used in concrete, Cement and Concrete Research, 2002, 32, 1621-1638