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Mesoscale modeling of fracture in cement and asphalt concrete

Key words: mesoscale model, damage model, fracture energy, cement concrete, asphalt concrete, disk-shaped compact tension test

Introduction

Numerical modeling of concrete materials has taken several paths over the years. The most common method is macroscale modeling where concrete is modeled as a homogenous material. This type of modeling has two distinct approaches: continuum models and fiber-based models. Continuum models are the most commonly used type which utilize commercial finite element programs and they are computationally expensive. Fiber-based models, on the other hand, are less common and not computationally costly (Al-Jelawy, 2017; Haber, Mackie & Al-Jelawy, 2017; Al-Jelawy, Mackie & Haber, 2018). Recently, an-

other type of modeling has emerged which is the mesoscale modeling.

Mesoscale modeling has become an alternative modeling method for macroscale modeling for the simulation of heterogeneous materials such as cement and asphalt concrete since realistic damage prediction and crack growth are crucial aspects of such materials (Unger, Eckardt & Koenke, 2011; Thilakarathna, Baduge, Mendis, Vimonsatit & Lee, 2020). Mesoscale modeling in cement or asphalt concrete requires aggregate and mortar to be modeled as separate constituents. Sometimes an interfacial transition zone (ITZ) between the aggregate and mortar is modeled as a third material (Unger & Eckardt, 2011).

Heterogeneous material is created using image processing techniques or through random generation of aggregates. Aggregate can be rounded in shape or having sharp angles. Aggregate

size distribution is modeled through prescribed curves or empirical equations such as Fuller curve (Häfner, Eckardt, Luther & Könke, 2006; Zhang, Song, Liu, Wu & Song, 2017). Material models are then assigned to the aggregate and mortar based on their individual properties.

In previous studies, continuum models such as smeared crack models, damage models, and plastic-damage models were used to represent fracture properties within the numerical model (Unger & Eckardt, 2011). Also, models which utilized discrete cracks implemented in rigid-body-spring model were used (Grassl & Bažant, 2009), or discrete cracks which were included in finite elements such as extended finite elements (Moës, Dolbow & Belytschko, 1999).

Recently, the use of mesoscale modeling has been limited to simulate specimen subject to tension (Kim & Al-Rub, 2011; Unger & Eckardt, 2011; Unger et al., 2011; Chen, Xu, Mo & Zhou, 2018; Zhou & Lu, 2018; Karavelić, Nikolić, Ibrahimbegovic & Kurtović, 2019; Jin, Yu, Du & Yang, 2020) and compression (Xie, Guo, Yuan & Huang, 2015; Chen et al., 2018; Zhou & Lu, 2018; Karavelić et al., 2019; Chen et al., 2020). The use of fracture mechanics in civil engineering have restraints related to the selection of the test specimen geometry and the available equipment to run the test. The common specimen geometry used for concrete fracture testing is the three-point notched beam. Specimens extracted from the field have become more desirable in order to evaluate in situ structure capacity. Therefore, concrete cores are a suitable option for

fracture testing since extracting beams from the field is difficult. Recently, geometry selection for concrete (Amirkhanian, Spring, Roesler & Paulino, 2016) was motivated by previous research on asphalt concrete specimens (Wagnoner, Buttlar & Paulino, 2005; Wagnoner, Buttlar, Paulino & Blankenship, 2006; Kim, Buttlar, Baek & Al-Qadi, 2009) where a disk-shaped compact tension test (DCT) was used extensively on asphalt core specimens that gave consistent and accurate results. Later the DCT geometry was adopted for asphalt specimens as a standard in ASTM D7313 (ASTM International [ASTM], 2013). The main advantage of the DCT specimen geometry is the easy fabrication from a field core or laboratory cylinder. Numerical studies that are performed on cement and asphalt DCT tests are mainly in macroscale (Wagnoner et al., 2005; Amirkhanian et al., 2016). Only one mesoscale study was conducted on mesoscale asphalt concrete specimens (Kim et al., 2009), while none were implemented on cement concrete DCT tests.

The objective of this study is to perform a mesoscale analysis on DCT specimens of cement concrete and asphalt concrete in order to obtain more realistic behavior of these heterogeneous materials. In mesoscale models, aggregate and matrix are represented as distinct materials and each material has its characteristic properties. Experimental data from previous studies on DCT specimens were used to validate the modeling results in terms of load-crack mouth opening displacement (CMOD) relationship.

Material models

Material models for fracture mechanics are mainly two types: constitutive models that represent cracks as a reduction in constitutive stiffness such as smeared crack model, damage models and damage-plasticity models. The other type of models such as embedded finite elements (Jirásek, 2000) and extended finite elements (Moës et al., 1999) utilizes a crack as a discontinuity in the displacement field. The first type of models has gained popularity due to its compatibility with finite element analysis (Rots, Nauata, Kuster Blaauwendraad, 1985; Rots, 1988; Rots & Blaauwendraad, 1989).

In the current study, isotropic damage model was used, and it is explained in the subsequent paragraphs. The softening curve for this model is defined as a function of fracture mechanics parameters.

This is the simplest form of damage models. It assumes that the damage is equal in all directions and represented by scalar value – ω (Kachanov, 1986; Le-maitre & Chaboche, 1990). The model is applied to the cementitious material only (such as cement mortar or asphalt) while the aggregate is modeled using its elastic properties.

The damage model is based on the following stress-strain relationship:

$$\sigma = (1 - \omega(\epsilon)) D_e \quad (1)$$

where D is the elastic material matrix. The damage (ω) can be defined as a function of fracture mechanics parameters as (Kurumatani, Terada, Kato, Kyoya & Kashiyama, 2016):

$$\omega(\epsilon) = \begin{cases} 1 - \frac{1}{E} \left(\frac{1}{\epsilon} \cdot \left(f_t - (f_t - \sigma_s) \cdot \frac{(\epsilon - \epsilon_0)}{w_s} \right) \right), \\ \text{if } (\epsilon - \epsilon_0) < w_s \\ 1 - \frac{1}{E} \left(\frac{1}{\epsilon} \cdot \left(\sigma_s \cdot \left(w_c - \frac{(\epsilon - \epsilon_0)}{w_c - w_s} \right) \right) \right), \\ \text{if } (\epsilon - \epsilon_0) \geq w_s \text{ and } (\epsilon - \epsilon_0) < w_c \\ 1, \quad (\epsilon - \epsilon_0) \geq w_c \end{cases} \quad (2)$$

Equation (2) is for bilinear softening, other softening types have different equations. The damage (ω) is zero if $\epsilon < \epsilon_0$.

Where:

E – elastic modulus of the concrete or asphalt mortar material,

f_t – uniaxial tensile strength of the concrete or asphalt mortar material,

σ_s – stress at the point of slope change of bilinear softening curve, $\sigma_s = 0.25 f_t$,

w_s – damage at the point of slope change of bilinear softening curve, $w_s = 0.15 w_c$.

w_c – damage occurs at critical crack width. It can be defined as:

$$w_c = 5 \frac{G_f}{h f_t} \quad (3)$$

Where G_f is the total fracture energy of the mortar material and h is equivalent element size defined as:

$$h = \sqrt{A_e}$$

for quadratic elements and:

$$h = \sqrt{2A_e} \quad (5)$$

for triangular element where A_e is the element area. ϵ_0 is the cracking strain and defined as:

$$\epsilon = \frac{f_t}{E} \quad (6)$$

ϵ is the highest equivalent strain the material ever experienced and related to equivalent strain ϵ_{eq} in case of loading and unloading as:

$$\epsilon_{eq} > \epsilon \Rightarrow \epsilon = \epsilon_{eq} \text{ (loading)} \quad (7)$$

$$\epsilon_{eq} \leq \epsilon \Rightarrow \epsilon = \epsilon \text{ (unloading)} \quad (8)$$

Equivalent strain is defined as:

$$\epsilon_{eq} = \sqrt{\epsilon_{1b}^2 + \epsilon_{2b}^2} \quad (9)$$

Where:

$$\epsilon_{1b} = \epsilon_1 \text{ if } \epsilon_1 > 0 \text{ otherwise } \epsilon_{1b} = 0 \quad (10)$$

$$\epsilon_{2b} = \epsilon_2 \text{ if } \epsilon_2 > 0 \text{ otherwise } \epsilon_{2b} = 0 \quad (11)$$

Where ϵ_1 and ϵ_2 are major and minor principal strains. It has been shown that isotropic damage model has low mesh sensitivity than other models such as smeared crack models (Kurumatani et al., 2016).

Geometry generation

To obtain a realistic representation of the concrete structure, the shape and size distribution of aggregate are described using a grading curve. Grading curves

(4) can be obtained using empirical equations such as Fuller curve. In the current study, Fuller curve was used which is in the following form:

$$passing = \left(\frac{d}{d_{max}} \right)^\alpha \cdot 100 \quad (11)$$

where

d – sieve size [mm],
 d_{max} – maximum size of aggregate [mm],

$passing$ – accumulated percentage that pass the sieve size [%],
 α – Fuller curve exponent and assumed to equals to 0.45 in the current study. Figure 1a shows an example of actual and simulated aggregate distribution using Fuller curve.

After that, ellipsoids are generated in three-dimensional domain (refer to Fig. 1b). Each individual ellipsoid has dimensions which are determined from the sieve curve and aspect ratio of the required aggregate. Aggregates are placed according to algorithm commonly known as set and place method which is explained by Unger et al. (2011). Based on this algorithm, the particles are divided into sets based on their sizes and then placed individually. If the placed particle intersects with another particle it will be placed again in a different empty spot. After particle placement was done, the ellipsoids were cut by a plane to obtain ellipses to shift the focus on two dimensional problems (refer to Fig. 1c). The cutting plane is located in the middle of width direction to avoid underrepresentation of larger particles near the edges of the specimen. Afterwards, specimen was

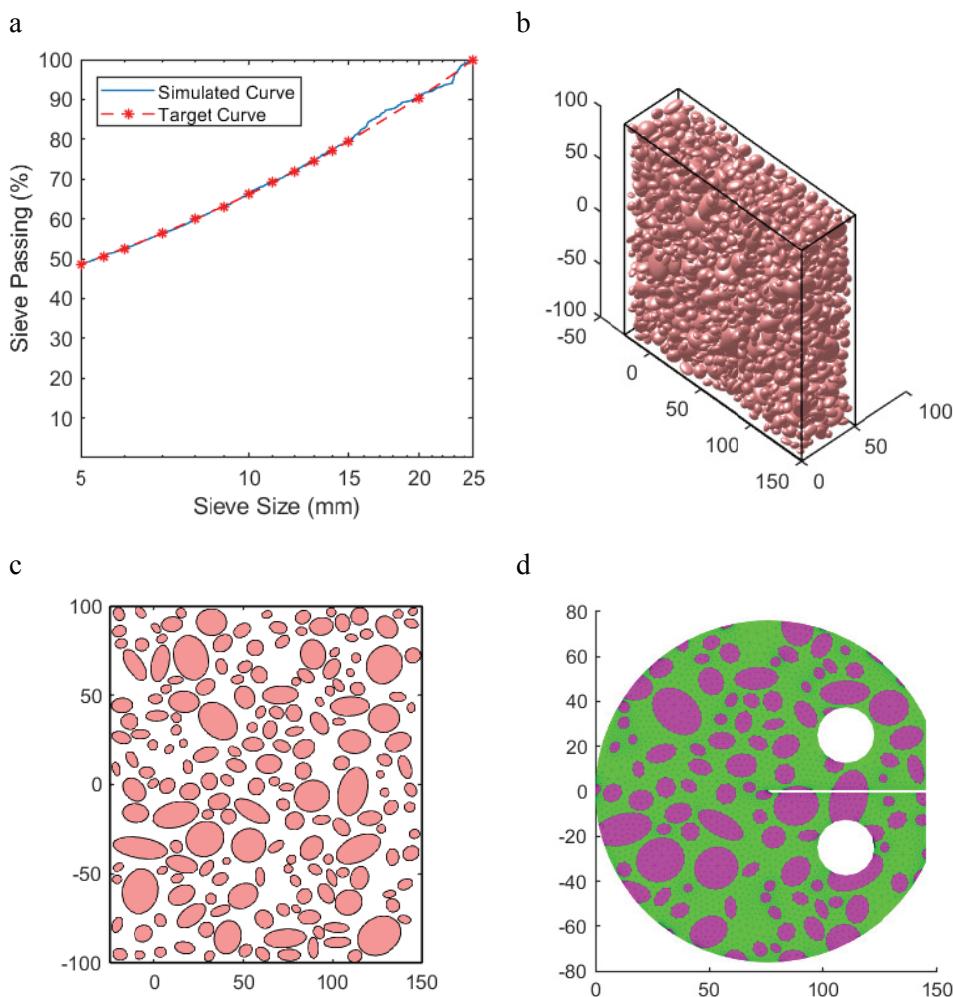


FIGURE 1. Geometry generation steps: a – sieve analysis; b – ellipsoids; c – ellipses; d – mesh

cut to form a disk-shaped geometry similar to that used in DCT test and a notch was made (see Fig. 1d). The ellipses were allowed to be cut at the boundaries to simulate in-situ conditions. Triangular mesh based on Delaunay triangulation was generated using MESH2D MATLAB code for two-dimensional geometries (Engwirda, 2005, 2014).

Numerical solution method

Cement and asphalt concrete tests were simulated using finite element method, and the triangular mesh was modeled as constant strain triangles elements. The applied load was vertical static support displacement through the circular holes with additional horizon-

tal support to ensure translational and rotation stability. The non-linear behavior was solved using Newton Raphson method with line searches implemented in MATLAB. The analysis results were compared with available experimental data in subsequent sections.

Model validation with Portland cement concrete experiments

The numerical model was validated against experimental tests of disk-shaped tension tests of concrete specimens. The selected specimens were tested by Amirkhanian et al. (2016). The material average properties are given in Table 1. They were 24 cored specimens, 18 specimens were tested at age 710 days (referred to as Mortar 1 in Table 1) and 6 specimens were tested at 1,578 days (Mortar 2 in Table 1). The averaged curves of the two types of the specimens were used in the comparisons with the numerical model.

Limestone coarse aggregate was used in all specimens with grading size of 5–20 mm. The percentage of coarse and fine aggregate was assumed 75% by volume. Fuller curve exponent of 0.45 was adopted. Aggregate distribution for the two types of specimens (Mortar 1 and Mortar 2) is shown in Figure 2a and Figure 3a, respectively. Disk geometry for the two types of specimens is shown in Figure 2b and Figure 4b, respectively. Crack growth from numerical simulation is shown in Figure 2c and Figure 3c for the two types. It can be observed that crack initiation and propagation are more realistic than straight cracks in macroscale models. The relationship between load and CMOD for the two types of specimens from numerical analysis is comparable to that from the experiments as depicted in Figure 2d and Figure 3d, respectively. The numerical model is able to predict the tensile strength, initial stiffness and the softening branch of load-CMOD curve with good accuracy.

TABLE 1. Material properties for cement concrete specimen

Aggregate	E [MPa]	ν	f_t [MPa]	G_f [$N \cdot mm^{-1}$]
	45 000	0.2	—	—
Mortar 1	38 000*	0.2	4**	0.15**
Mortar 2	38 000*	0.2	4.62***	0.163***

*Mortar modulus of elasticity was chosen in order to achieve bulk modulus of elasticity 40,600 MPa by using the following equation based on Reuss formula (Reuss, 1929):

$$E_{\text{bulk}} = \frac{100}{\frac{\% \text{ aggregate}}{E \text{ aggregate}} + \frac{\% \text{ mortar}}{E \text{ mortar}}} \quad (12).$$

**Tensile strength in macroscale model was 4 MPa and fracture energy is 0.1252 MPa.

***Tensile strength in macroscale model was 4.2 MPa and fracture energy is 0.148 MPa.

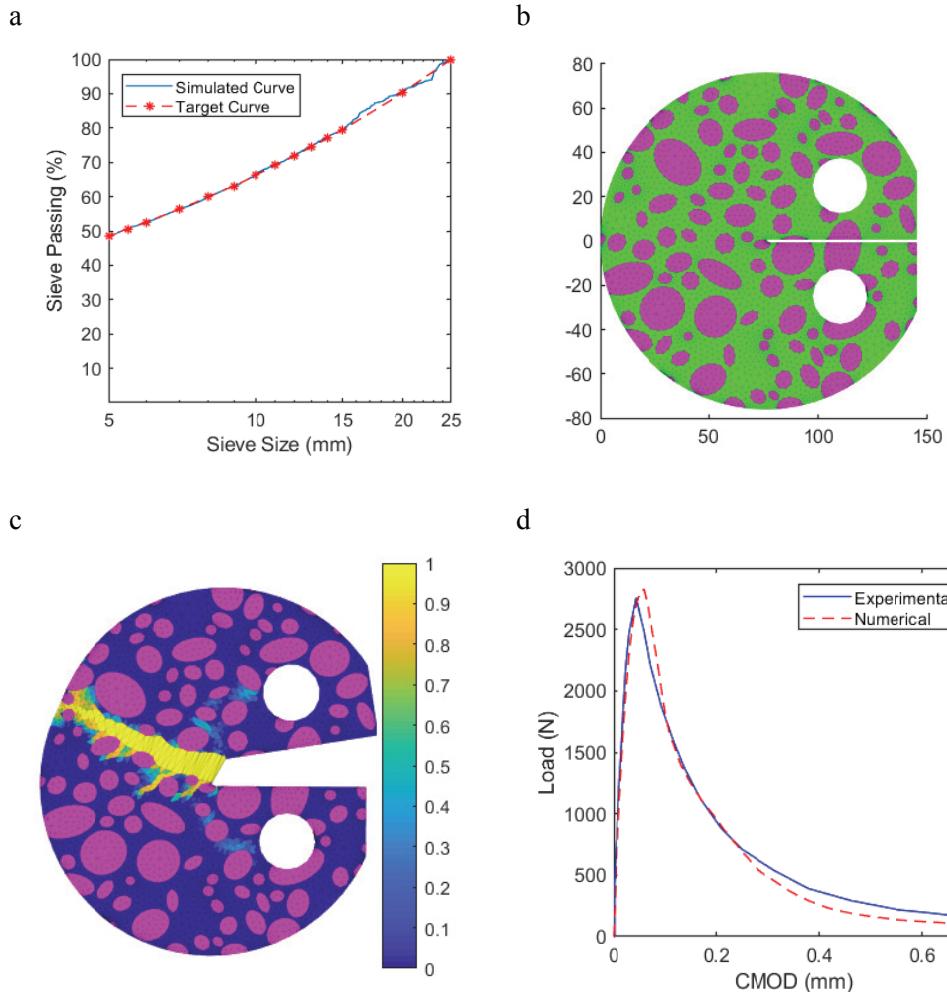


FIGURE 2. Model validation for cement concrete DCT (Mortar 1) specimens: a – sieve analysis; b – cement concrete mesh (7,028 elements); c – crack path at failure; d – load-CMOD curves

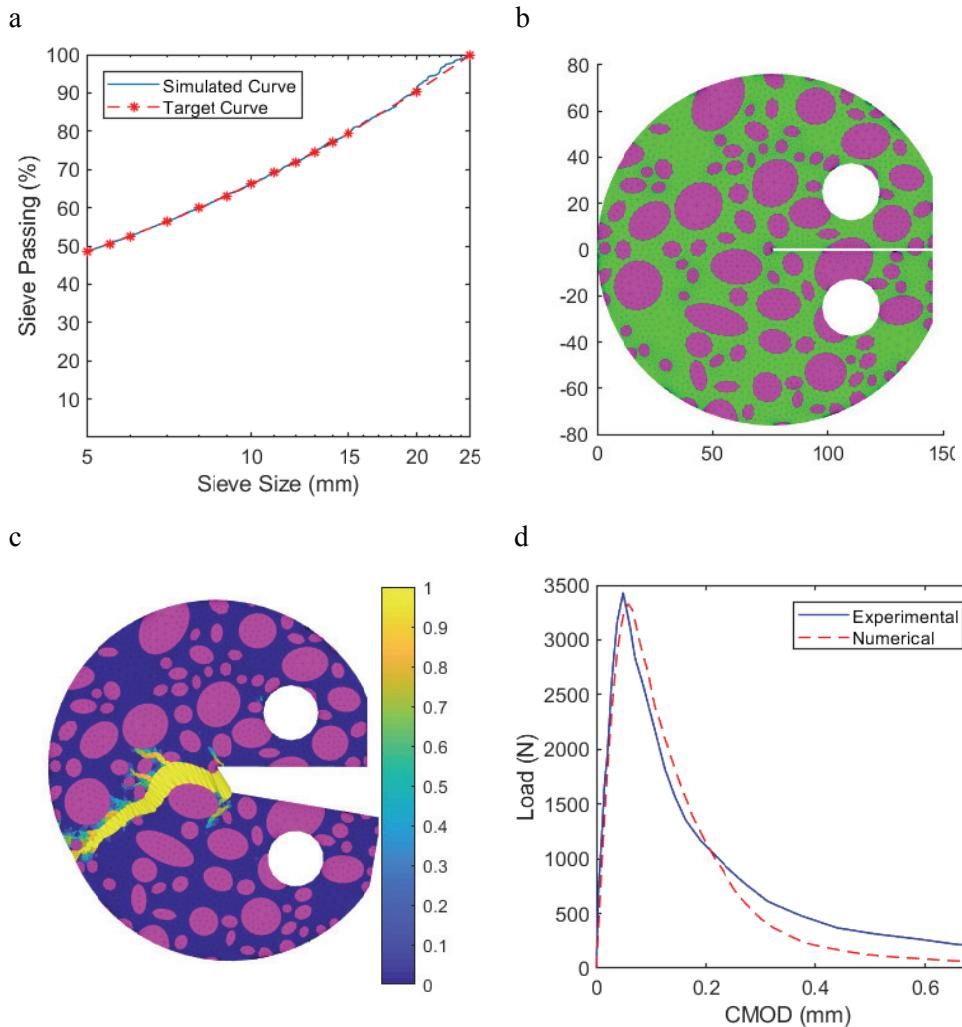


FIGURE 3. Model validation for cement concrete DCT (Mortar 2) specimens: a – sieve analysis; b – cement concrete mesh (8,082 elements); c – crack path at failure; d – load-CMOD curves

Comparisons with asphalt concrete experiments

In addition to the concrete specimens, of disk-shaped tension tests of asphalt specimens were used to validate the proposed numerical model. Three

specimens were tested by Wagnoner et al. (2005). One mix was used with aggregate of grading size of 5–9.5 mm and an asphalt binder. Percentage of aggregate was assumed to be 90% by volume. Fuller curve exponent of 0.45 was adopted. Aggregate distribution of the

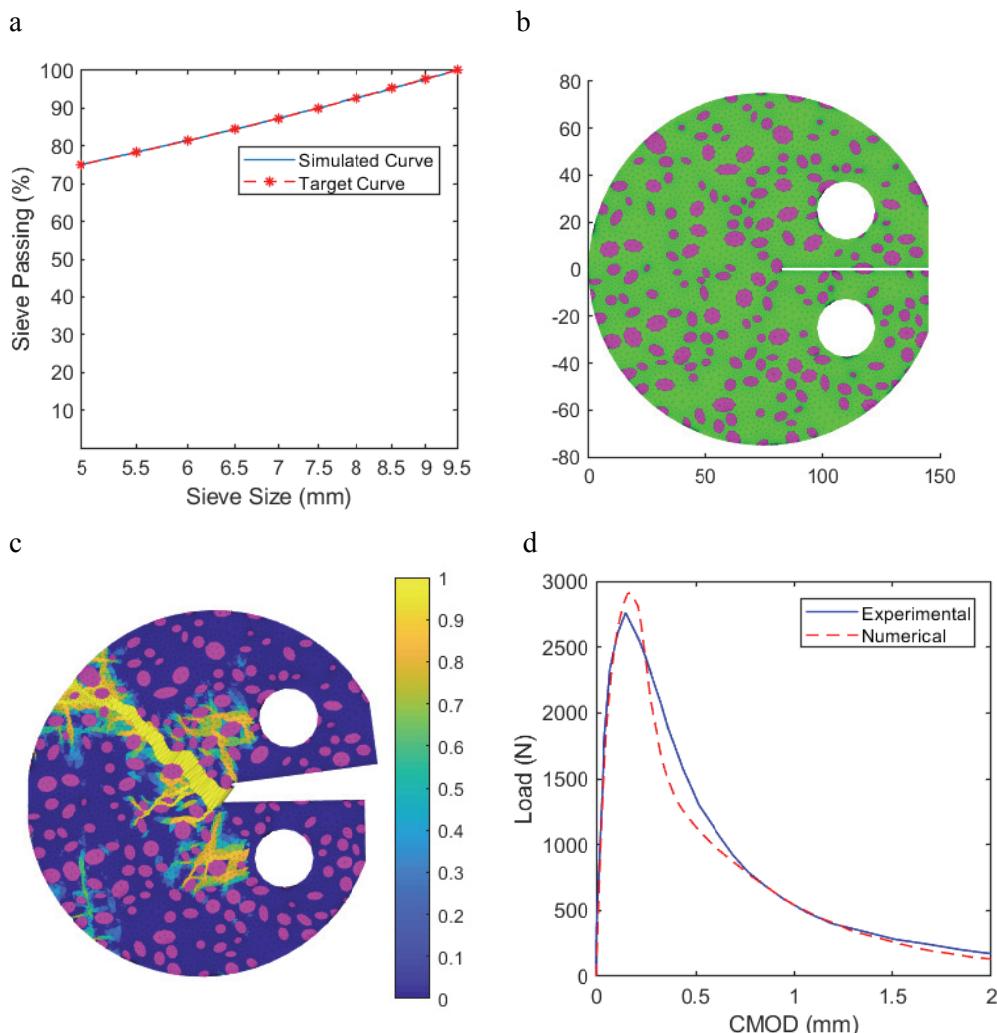


FIGURE 4. Model validation for asphalt concrete DCT specimens: a – sieve analysis; b – asphalt concrete mesh (14,708 elements); c – crack path at failure; d – load-CMOD curves

specimens is shown in Figure 4a. Disk geometry of specimens is shown in Figure 4b. The failure mode of the specimen from the numerical modeling is shown in Figure 4c. It can be seen that crack initiation and propagation are similar to that in an actual asphalt concrete specimen.

Also, the numerical load-CMOD curve is in agreement with the experimental curve as depicted in Figure 4d. The predicted tensile strength, initial stiffness and the softening branch of load-CMOD curve are comparable to the experimental results.

TABLE 2. Material properties for asphalt concrete specimen

Material	E [MPa]	ν	f_t [MPa]	G_f [$N \cdot mm^{-1}$]
Aggregate	50 000	0.2	—	—
Mastic	12 000*	0.35	2.85**	0.459**

*Mastic modulus of elasticity was chosen in order to achieve bulk modulus of elasticity 14,200 MPa by using the following equation based on Reuss formula (Reuss, 1929):

$$E_{\text{bulk}} = \frac{100}{\frac{\% \text{ aggregate}}{E \text{ aggregate}} + \frac{\% \text{ mastic}}{E \text{ mastic}}} \quad (13)$$

**Tensile strength chosen 80% of indirect tensile splitting test results, while in the macroscale model of the original paper it was 74%. Fracture energy value in macroscale model is 0.328.

Conclusions

In this study, mesoscale modeling is performed on fracture behavior of cement and asphalt concrete composites using disk-shaped compact tension (DCT) tests. Realistic behavior of composite and heterogeneous materials such as cement and asphalt concrete require mesoscale modeling. In the presented model, aggregate and matrix (cement mortar or asphalt) are represented as distinct materials and each material has its characteristic properties where the matrix is modeled using isotropic damage model with softening and the aggregate is modeled using its elastic properties. Disk-shaped compact tension test is a better alternative to other tests such as three points bending tests for the determination of tensile strength and fracture energy of materials because it is more convenient for both field and laboratory specimens in addition to its accurate results. The test geometry is generated using a MATLAB code that takes care of the shape and size distribution

of the aggregate. The numerical results show that the predicted load-CMOD curves are in good agreement with the experimental curves for both cement and asphalt concrete. Also, the numerical model can capture the variability of crack direction very well.

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- istic properties. Disk-shaped compact tension test is used to obtain tensile strength and fracture energy of materials. This test can be used as a better alternative to other tests such as three points bending tests because it is more convenient for both field and laboratory specimens in addition to its accurate results. Comparing the numerical results of the mesoscale models of cement and asphalt concrete specimens with experimental data shows that these models can predict the behavior of these composite materials very well as seen in the curves of load-crack mouth opening displacement (CMOD). Also, the mesoscale modeling highlights the variability of crack direction where it is dependent on the random distribution of aggregate.

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Summary

Mesoscale modeling of fracture in cement and asphalt concrete. In this paper, mesoscale modeling is performed to simulate and understand fracture behavior of two concrete composites: cement and asphalt concrete using disk-shaped compact tension (DCT) tests. Mesoscale models are used as alternative to macroscale models to obtain better realistic behavior of composite and heterogeneous materials such as cement and asphalt concrete. In mesoscale models, aggregate and matrix are represented as distinct materials and each material has its character-