



Research Paper

A calibration methodology to obtain material parameters for the representation of fracture mechanics based on discrete element simulations



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ABSTRACT

A micro-mechanical model is developed to study the fracture propagation process in rocks. The model is represented by an array of bonded particles simulated by the discrete based method. Experimental results of tests using Cracked Chevron Notched Brazilian Discs (CCNBD) with different inclination angles relative to the direction of loading are used to calibrate and validate the model. Dimensional analysis is used to identify and minimise the microscale parameters to be considered. The comparison between experimental and computational results shows a satisfactorily good agreement.

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1. Introduction

Predicting the failure load in brittle materials such as rocks that contain pre-existing cracks, and determining the effect of the load and crack geometry on failure, are important in the design of structures in such materials. In order to study the failure process, the prediction of the trajectory of crack growth in the brittle material is an important question that needs to be addressed.

Since the fracture process is in principle discontinuous, the Discrete Element Method (DEM) is considered to be an appropriate numerical approach to investigate the fracture processes in rocks. The use of continuous approaches such as the finite element or finite difference methods for studying the fracturing process in rocks may assist in assessing the weakening zone, but will not allow the quantitative determination of the fracture geometry during crack propagation, after fracture initiation. In fact, in continuum-based methods, the behaviour of discontinuous zones is not well described [1]. Among the discrete numerical techniques, the most effective and simple to apply to the crack propagation

process in rock would be considering clusters of discrete particles in contact that are connected by cohesive or bonding forces. Even though cohesive forces have different physical origins, they all have the same effect, which is resisting the relative displacement that can occur between particles up to the time when they reach the threshold value [2]. In this paper, DSEM (Discrete Sphero-Polyhedra Element Model) is used to model sphero-polyhedral-shaped particles extracted from Delaunay tessellations [3]. This is a departure from the traditional spherical element DEM approach and allows to model solid bodies without any internal voids. This DSEM technique has proven to be a very versatile discrete technique able to simulate non-convex shapes [4], fracture processes [2], and even the interaction between complex-shaped bodies and fluids [5].

When rock with a pre-existing crack is subjected to external loading forces, stresses concentrate at the crack tip. If these stresses exceed the threshold value, the crack starts to propagate resulting in rock failure. Depending on the direction of the applied load regarding the pre-existing crack, a crack propagates through by one of three different modes (modes I, II and III) or mixed mode [6]. Mode I is the tensile opening mode, resulting in normal stresses applied at the crack tip and lead to the opening the crack. Mode II is the in-plane sliding or shearing mode, acting in the direction of

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crack extension. Mode III is tearing, or the anti-plane mode, in which the crack surfaces shear relative to each other. In fact in rock samples mode I, mode II and mixed mode are more common [6]. Different experimental and mathematical studies have been conducted to investigate the mechanism of crack growth under different levels of loading [7–18,22].

In 1995, the International Society for Rock Mechanics (ISRM) presented the CCNBD test procedure to determine the mode I fracture toughness in rock [23], that the geometry of CCNBD samples varies in a valid range. In rock mechanics, fracture toughness is the fundamental parameter related to the materials resistance to fracture propagation from a pre-existing crack. In literature the CCNBD test is used for determining mixed-mode fracture toughness by changing the inclination angle of the crack with respect to the direction of loading [10–12,14,15,17,18,22].

In the present study, CCNBD samples are simulated to validate DSEM approach for studying the macroscopic behaviour of specimens subjected to static loading, with the crack opening displacement measured as a function of crack inclination. The measured crack opening displacement was successfully simulated using the DSEM. This is achieved by using dimensional analysis to derive relationships between the microscopic parameters and the macroscopic responses and using those relationships to calibrate the DSEM. Finding the microscopic parameters which affect the crack propagation has never been investigated before. Also, the breakage of the specimens at the micro-scale is studied and an open question is proposed on how to connect the micro-damage with the macroscopic modes used in continuous models.

In Section 2 of the paper, the experimental studies and results are reviewed. Section 3 includes an explanation of the simulation set-up and the numerical modelling of the CCNBD specimens using the DSEM method. This section includes some discussion and comparisons between both experimental and numerical results. Section 4 presents the conclusions.

2. Experimental study

The CCNBD test was suggested in 1995 by the ISRM for measuring the fracture toughness of mode I (tensile) fractures [23]. A CCNBD specimen is a Brazilian disc with a notch cut using a circular saw from both sides in the middle of the specimen. By applying a compressive load across the circumference of the disc, a crack initiates and propagates from the notch towards the boundary of specimen. Fig. 1 illustrates the geometry of a CCNBD specimen used in the experiments [24]. The radius of disc (R) is 26 mm and the thickness of specimens (T) is 24 mm. The inner chevron notched crack length ($2a_0$) is 15 mm and the outer chevron notched crack length ($2a_1$) is 38 mm. In the specimens considered for this study, the thickness of the notch is 1.5 mm. A circular 40 mm diamond saw is used to cut the notch ($2R_s$). In CCNBD test, by changing the direction of loading relative to the crack inclination, different fracture modes including a mixed fracture mode can be obtained [10–12,14,15,17,18,22].

For the specimens with pre-existing crack, the stresses at the crack tip can be tensile or shear depending on the crack inclination angle. Tensile stresses, in combination with shear stresses at the crack tip, cause a crack that propagates in a variety of mixed modes I and II failure trajectories. In the experimental studies reported in [24], CCNBD specimens were cut and then pure mode I and a range of mixed-mode loading conditions were investigated.

2.1. Experiments for determination of mixed-mode fracture of rocks

In the experiments described in [24], CCNBD specimens were prepared from cores of Brisbane tuff and tested with various crack inclinations. The tests were carried out on different rock samples

with mean Poissons ratio of 0.24, Young's modulus of 22 GPa, uniaxial compressive strength of 101 MPa and tensile strength of 11.5 MPa [17,24].

In these tests, displacement was controlled and increased with a constant rate until failure occurred. The inclination angles of the loading direction to the notch crack (β) tested were as $0^\circ, 28^\circ, 30^\circ, 33^\circ, 45^\circ$ and 70° [17,24]. During the experiments, the load and CMOD were recorded continuously. The compressive loads induced both tensile and shear stresses in the notch crack in the CCNBD specimens. During loading process, the crack initiates in Mode I and propagates in the direction parallel to the orientation of the compressive loading [25].

Fig. 2 shows the measured load versus CMOD (Crack Mouth Opening Displacement) plots at different inclination angles (β) for Brisbane tuff CCNBD specimens [24]. As can be seen in Fig. 2, depending on the inclination angle the crack can close or open further. When the crack is parallel to the loading direction, the fracture initiates at the ends of the notch, while when it is perpendicular, the fracture initiation moves towards the middle of the notch [17,24]. Furthermore, opening occurred for $\beta \leq 30^\circ$ while closing occurred for $\beta > 33^\circ$, but for β between 30° and 33° both opening and closing displacements were observed. In these experiments, the maximum applied load was approximately 5 kN [17,24].

Mode I stress intensity factor and fracture toughness for CCNBD samples when $\beta = 0$, can be calculated from ISRM suggested method [23] by Eq. (1)

$$\begin{aligned} \text{Mode I stress intensity factor } K_I &= \frac{P}{T\sqrt{R}} Y^* \\ \text{Mode I fracture toughness } K_{IC} &= \frac{P_{max}}{T\sqrt{R}} Y_{min}^* \end{aligned} \quad (1)$$

where P is the applied loading force and P_{max} is the failure load; Y^* represents the dimensionless stress intensity factor that is a function of sample geometry and Y_{min}^* is the minimum dimensionless stress intensity factor as it corresponds to the failure load; T and R are the thickness and radius of sample respectively. However, there is no suggested methods by the ISRM for determining the mixed mode stress intensity factor and fracture toughness for CCNBD tests with different direction of pre-existed crack. For studying mixed mode fracture toughness and stress intensity factor Cracked Straight Through Brazilian Disc (CSTBD) is used. In 1985 Sheity et al. [26] suggested a formula to find fracture toughness of CSTBD samples with the length of straight through crack $2a$ (Eq. (2)).

$$\begin{aligned} \text{Mode I stress intensity factor for CSTBD } K_I &= \frac{P}{T\sqrt{\pi R}} \sqrt{\alpha} N_I \\ \text{Mode II stress intensity factor for CSTBD } K_{II} &= \frac{P}{T\sqrt{\pi R}} \sqrt{\alpha} N_{II} \end{aligned} \quad (2)$$

In Eq. (2), N_I and N_{II} are the dimensionless stress intensity factors depending on the dimensionless crack length ($\alpha = a/R$) and the crack inclination angle with respect to the loading direction β . N_I and N_{II} solutions have been provided by Atkinson et al. [27] Sheity et al. [26] and Fowell and Xu [28].

Chang et al. proposed in 2002 two different equations to find stress intensity factor for CCNBD samples in mode I and mode II (Eq. (3)) by applying Eq. (2) and by substituting T (thickness of sample) to $T \times \sqrt{\alpha - \alpha_0} / \sqrt{\alpha_1 - \alpha_0}$ that includes geometry of notch in CCNBD samples (initial and final chevron notched crack length) (Eq. (3)) [11].

$$\begin{aligned} \text{Mode I stress intensity factor for CCNBD } K_I &= \frac{P}{T\sqrt{\pi R}} \sqrt{\alpha} \sqrt{\frac{\alpha_1 - \alpha_0}{\alpha - \alpha_0}} N_I \\ \text{Mode II stress intensity factor for CCNBD } K_{II} &= \frac{P}{T\sqrt{\pi R}} \sqrt{\alpha} \sqrt{\frac{\alpha_1 - \alpha_0}{\alpha - \alpha_0}} N_{II} \end{aligned} \quad (3)$$

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