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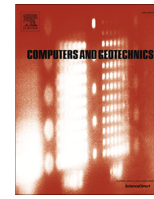

Discrete element simulation of the effect of particle size on the size of fracture process zone in quasi-brittle materials

Ali Tarokh [a,*], Ali Fakhimi [b,c]

[a] Department of Civil Engineering, University of Minnesota, Minneapolis, MN 55455, USA
[b] Department of Mineral Engineering, New Mexico Institute of Mining and Technology, Socorro, NM 87801, USA
[c] School of Civil and Environmental Engineering, Tarbiat Modares University, Tehran, Iran

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A B S T R A C T

Experimental tests performed on quasi-brittle materials show that a process zone develops ahead of a crack tip. This zone can affect the strength and the deformation pattern of a structure. A discrete element approach with a softening contact bond model is utilized to simulate the development of the fracture process zone in the three-point bending tests. Samples with different dimensions and particle sizes are generated and tested. It is shown that as the material brittleness decreases, the width of the process zone becomes more dependent on the specimen size. Furthermore, the increase in the particle size, results in increase in the width of the process zone. A dimensional analysis together with the numerical results shows that the width of process zone is a linear function of particle size (radius). This finding is discussed and compared with published experimental data in the literature.

1. Introduction

Structures composed of quasi-brittle materials such as rock or concrete exhibit a zone of localized microcracking when the strength of the material is approached. The estimation of the material strength has been shown to be dependent on this localized zone and the structure itself [1,2]. Furthermore, it has been experimentally observed that the path of the visible fracture is within this localized zone of microcracking [3,4]. Therefore, in modeling the response of a quasi-brittle structure, the characteristics of this localized zone or the so-called fracture process zone should be considered in predicting the tensile failure. Many researchers have shown significant interest in experimental investigation of the governing parameters affecting the fracture process zone. Some of the parameters that have been reported to influence the process zone are the specimen size [3,5], crack length [6], porosity [7,8], and loading rate [9]. Microstructure is also known to have a strong influence on the size of process zone [10–13]. Despite the qualitative observations of the influence of microstructure on the size of the process zone, a few quantitative relationships have been proposed. Zietlow and Labuz [3] suggested an approximate linear relationship between the width of the process zone and the logarithm of grain size. Mihashi and Nomura [14] studying the process zone in concrete by means of acoustic emission found that the length of process zone is independent of the maximum aggregate size but the width of the process zone is strongly affected. Wang et al. [15] investigated the influence of grain size on size of the process zone using laser speckle interferometry and reported that the size of the process zone is influenced by the ratio of notch width to the average grain diameter; if this ratio decreases, the size of process zone will increase. Otsuka and Date [5] implemented three dimensional acoustic emission and X-rays using contrast medium on concrete and found that with the increase of maximum aggregate size, the width and length of the process zone increase and decrease, respectively.

To investigate the effect of particle size on the width of the process zone, the bonded-particle model (BPM), which is based on the discrete element method (DEM), is adopted in the present work. A tensile softening contact bond model is used to mimic the development of the process zone. By varying the particle size and the material brittleness, different synthetic quasi-brittle samples were generated. The material brittleness was modified by changing the slope of the softening line (K_{np}). The samples were numerically tested in the three-point bending tests. It is shown that the increase in the particle size will increase the width of the process zone. Furthermore, it was found that the width of the process zone is a linear function of the particle size. For a fixed specimen size and notch length, the increase in the particle size will result in a larger process zone making the material less brittle.

* Corresponding author. Tel.: +1 612 625 8337.
E-mail address: tarok001@umn.edu (A. Tarokh).

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2. Numerical model

In this paper, the CA2 computer program, which is a hybrid discrete-finite element program for two-dimensional analysis of geomaterials, was used to simulate the failure process in Berea sandstone [16–18]. The bonded-particle model [19], which is one of the discrete element method (DEM) based particle models has been used extensively for simulating rock failure [20,21]. The rock is modeled as a bonded particle system in which the rigid circular particles (representing the grains) interact through normal and shear springs to simulate elasticity. Rigid particles mean that they maintain their shape while they can slightly overlap at the contact points in reaction to the applied stresses. When rigid particles are used, only translation of the centroids and the rigid body rotation of the particles need to be considered in the simulation, i.e. there are three degrees of freedom for a two dimensional particle. If the particles could deform (not rigid), then the particle deformations (strains) would need to be included in the governing differential equations, effectively increasing the number of degrees of freedom in the system and the computational cost. Therefore, the assumption of the rigidity of the particles facilitates the simulation involving large number of particles (for the 320 × 960 mm rock beam of the simulated Berea sandstone, more than 1 million particles were used and a couple of weeks of computer time with an i7 processor were needed to finish the simulation). From physical point of view, application of rigid particles is justified when the particle rigidity is much greater than the binding material. Therefore, precise modeling of the particle deformation is not necessary to obtain a good approximation of the mechanical behavior [22]. Another simplification in our model is that the particle shapes are assumed to be circular. This assumption has given good results compared to many experimental observations [23,24]. Hogue [25] and Houlsby [26] present a comprehensive description of the issues associated with the choice of particle geometry in DEM. Finally, in the bonded particle models, it is assumed that the failure can only occur along the particle boundaries. The relative amount of different types of microcracks appears to depend on the mineralogy, rock type and stress state [27]. Hamil and Sriruang [28] found that the cracks propagate mostly along the grain boundaries in sedimentary rocks such as sandstone. On the other hand, in the crystalline rocks such as granite, transgranular paths were most frequent and sometimes dominant.

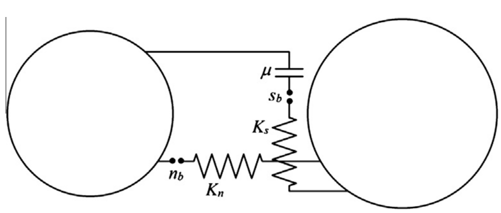

Fig. 1. Micro-mechanical constants involved for interaction of two circular particles.

In order to withstand tensile and deviatoric stresses, the rigid circular particles are bonded together at the contact points. Fig. 1 shows the micromechanical constants in this model. The micromechanical constants at a contact point in this model are K_n (normal stiffness), K_s (shear stiffness), n_b (normal bond), s_b (shear bonds), and μ (friction coefficient). In addition, the radius of the particles (R) must be specified. The genesis pressure (σ_0) that is the confining pressure during the sample preparation (determines the amount of initial small overlap between particles) can affect the material behavior too. The significance of these parameters has been discussed in a previous study [21].

Since quasi-brittle materials such as rock and concrete usually display tension softening during fracturing [29,30], a softening contact bond feature was implemented in the numerical model. In this softening model, the normal bond at a contact point is assumed to reduce linearly after the peak tensile contact load (Fig. 2a). Therefore, a new microscopic constant, the slope in the post peak region of the normal force-normal displacement between two particles in contact (K_{np}), is introduced in the model. As shown in Fig. 2b, no modification in the shear force-relative shear displacement of a contact is assumed in this simple model. Softening in shear is only relevant for loading under significant mean stress (more than 1/3 of uniaxial compressive strength). Distinct shear failure plane forms at moderate compression in which the mean stress, $p = (\sigma_1 + \sigma_2 + \sigma_3)/3$ is in the following range $\sigma_c/3 < p < \sigma_c$ [31]. This is not the case in the three point bending tests conducted in this study; no actual shear cracks are developed in our tests. The loading and unloading paths for both normal and shear contact forces are shown with arrows in Fig. 2.

After sample preparation, the numerical model was calibrated to obtain the mechanical properties of Berea sandstone. The procedures for sample preparation and calibration have been described elsewhere [21]. The grains in this particular sandstone range from 0.1 to 0.8 mm. The mechanical properties of the Berea sandstone are E (elastic modulus) = 14 GPa, ν (Poisson's ratio) = 0.32, σ_c (uniaxial compressive strength) = 55–65 MPa, and σ_N (bending tensile strength) = 8.6 MPa for an 80 × 240 × 30 (height × span × thickness) mm rock beam [3]. After calibration of the numerical model, uniaxial compressive test on an 40 × 80 mm (width × length)

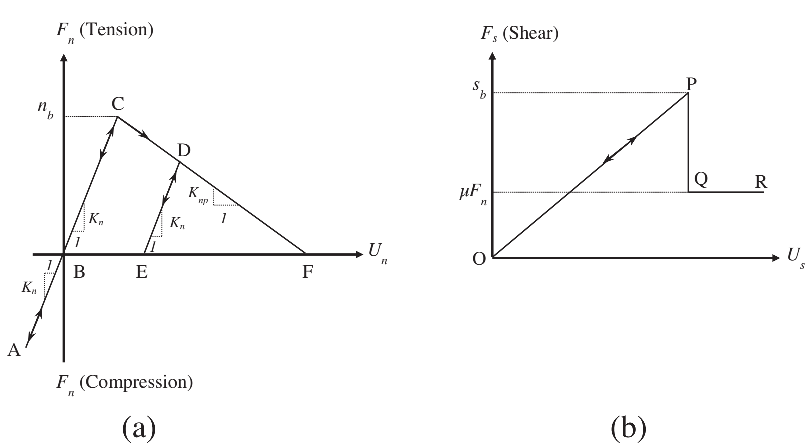

Fig. 2. Relationships in the softening contact bond model (a) normal force and normal displacement and (b) shear force and shear displacement [18].