Simulation of Hydro-Mechanical Coupling in 2D Bonded Particle Modeling

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1. INTRODUCTION

Many geophysical processes as well as a large number of geotechnical problems embody coupling between solid and fluid transfer and sometimes heat and reactive mass transfer must be considered as well. For example, high pore fluid pressure induces fracture development in rock masses and expansion of pore fluid by a nearby heat source results in openings of fractures or joints which reduces frictional resistance and consequently enhances the mobility of fault zones and jeopardizes the overall safety of the underground structures. Therefore, a basic understanding of rock mechanical properties under the presence of pore fluid pressure is necessary since many of the important problems of rock engineering are concerned with mechanical behaviors of rock where the internal rock structure sustains pore fluid pressure under confinement. Considerable attention has been given to the mechanical behaviors of rocks under different confining pressure and pore fluid pressure by laboratory tests and in-situ measurements, but the general theoretical formulations and laws of rock mechanical properties are still not formulated due to its extreme complexity. When a rock is subjected to stress, multiple cracks nucleate, propagate, interact and coalesce, which results in change of pore fluid pressure in the rock. This complex multiplicity of fracture interacting events also causes the complexity of mechanical breakdown of the rocks. Numerical model that are able to simulate the detailed fracturing of rocks combined with pore fluid pressure are thus necessary.

There have been several attempts for simulating solid-fluid coupling using various numerical schemes [1-3]. This paper deals with developing a coupling scheme between solid particles and pore fluids using commercial particle based modeling code, called Particle Flow Code 2D (PFC2D). Formerly the fluid flow algorithm in PFC was first proposed by Cundall [4] and later modified by Hazzard et al. [5]. Therefore, the objective of the present study is to modify the coupling algorithm and to apply to a biaxial compression simulation and see the variation of strength, fracturing, and seismic characteristics of cracking under the presence of pore fluid pressure. Results are analyzed and compared to the experimental findings various literature surveys.

2. INTERACTION OF SOLID PARTICLE AND PORE FLUID

2.1 Generation of pore fluid network

A compacted, bonded assembly of particles is generated first. A domain is defined as a closed chain of particles, such that each chain is a bonded contact. All domains are scanned to identify the complete set of domains for an assembly, so that the domains are scanned and accessible during the calculation cycle. Each domain element points to a local list of particles that surrounds the domain. For each bonded contact, a data block is created which contains pointers to the two domains that are adjacent to the contact. Fluid flow is simulated by assuming that each particle contact is a potential flow channel and that these channels connect up small reservoirs that store some fluid pressure. The channels join up and the fluid network is therefore continuous (Figure 1).

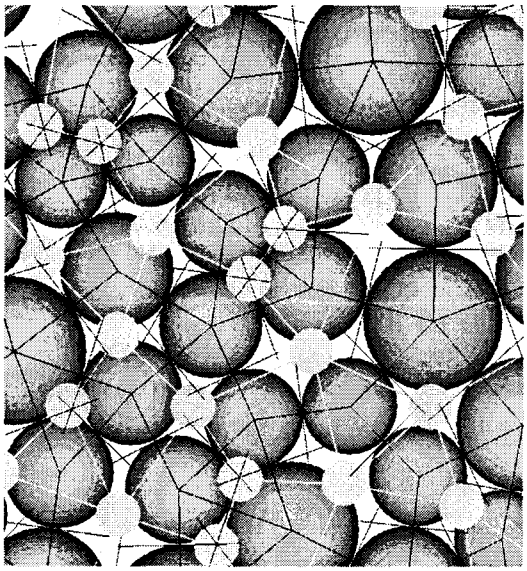

Fig. 1 Network of pore fluids (yellow dots) contained in voids between solid particles (gray dots). Fluid flows through the pipes denoted by red segments which are potential cracks that may break.

2.2 Formulation of fluid flow

Fluid formulation regards the void geometry in an assembly of particles as being identical to the actual space between particles. It is assumed that the assembly represents a material of low porosity, such as granite. Therefore, particles do not represent rock grains, but are simply means to

discretize space, and provide appropriate mechanical behavior, e.g. breakages of bonds, sliding, etc. Each pipe link between two adjacent domains is a potential crack, because it corresponds to a bonded contact that may break. Based on the former algorithms proposed by Cundall [4] and Hazzard et al. [5], some modifications have been made. The fluid flow algorithm assumes that the bonded particle model is made up of a series of channels through which fluid can flow. The volumetric flow rate through the pipes is calculated assuming laminar flow between two parallel plates having smooth surfaces. The equation is, therefore:

$$Q=\frac{a^3\Delta P}{12\mu L} \quad \text{--- (eqn.1)}$$

where, a is aperture, ΔP is pressure difference between domains, μ is dynamic viscosity of the fluid and L is length of a pipe. The aperture at a contact never decreases to zero. Instead, a residual aperture is specified that exists when the particles are just touching. The aperture, a, decreases asymptotically to zero as the compressive normal force, F, increases according to:

$$a=\frac{a_0F_0}{F+F_0} \quad \text{--- (eqn.2)}$$

where, a_0 is residual aperture and F_0 is force at which the aperture decreases to half of a_0. If the particles are not touching and some separation exists, then the aperture is set to the residual aperture a_0 and infinite permeability is assumed at the contact. This is necessary because pipes with large apertures lead to extremely small calculation time steps. Each domain receives flow from the surrounding pipes. In one time step, Δt, the change in fluid pressure is given by:

$$\Delta P=\frac{K_f}{V_d}\left(\sum Q\Delta t-\Delta V_d\right) \quad \text{--- (eqn.3)}$$

where, K_f is fluid bulk modulus and V_d is volume of domain. In sedimentary rock such as sandstone, the volume of the domain is assumed to be physical pore space defined by the grains making up the domain. This is estimated for each domain by calculating the area within the path joining the centers of particles comprising the domain and multiplied by the porosity. For crystalline rock such as granite, the pore space is assumed not to exist and the domain volume is set to one half of the sum of the pipe volumes entering into the domain (each pipe volume will be the pipe aperture times the pipe length times a unit thickness).

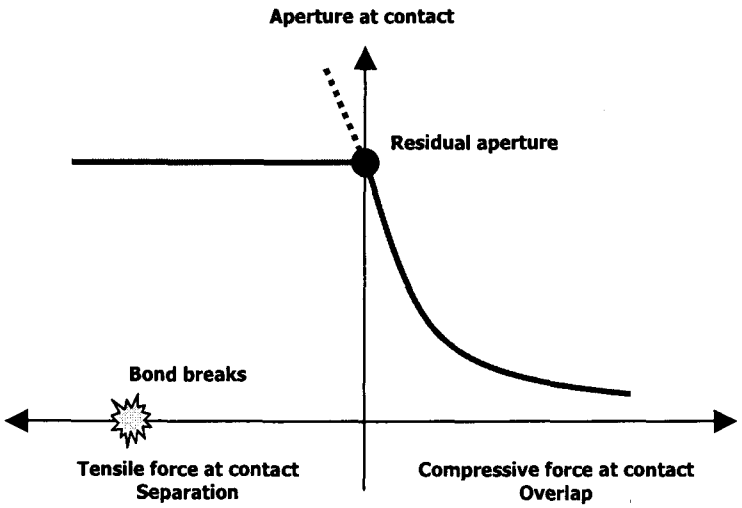

Fig. 2 Variation of aperture at contact. Residual aperture is defined as the aperture when the two particles are touching without any compression or tension.

For open pipes in which particles are not touching, equation 3 is bypassed and the pressure in each of the joined domains is set to the average pressure of the two domains. This essentially assumes that the pipe has an infinite permeability. This fluid flow algorithm is a modified form by Cundall [4]. The main modification done by Hazzard et al. [5] is that for open fractures (where the particles are not in contact), the fracture permeability is assumed to be infinite and the reservoir pressures on either side of the channel are set to a weighted average of the two pressures. This modification is necessary because otherwise open channels produce very high flow rates and calculations time steps must be very small to maintain numerical stability. Another modification implemented in this study is that when a contact is widely opened, then as the fluid flows through, it lubricates the surface of the particles so that they can slip without any resistance. Therefore, the program was made so that at the wide open contact the inter-particle friction coefficient reduces to zero.

2.3 Calculation of residual aperture

Darcy's law for a linear porous medium is expressed as:

$$q_i = -\frac{k_{ij}}{\mu}\frac{\partial P}{\partial x_j} \quad \text{--- (eqn.4)}$$

where, q_i is the one-dimensional flow rate (units of velocity), k_{ij} is the permeability and μ is dynamic viscosity of the fluid. The relationship between macro permeability and the

microparameters used in bonded particle model can be obtained by taking the volume average of flow contributions of all pipes within a control volume, V:

$$\bar{q}=\frac{1}{V}\sum_{pipes} q^p V^p \quad \text{--- (eqn.5)}$$

where, q^p is flow in a pipe, V^p is volume of a pipe and the summation is over all pipes in volume, V. The one-dimensional flow in a single pipe can be given by dividing volumetric flow in equation 1 by the pipe cross-sectional area A^p:

$$q^p=\frac{a^3 \Delta P n_i}{12\mu L A^p} \quad \text{--- (eqn.6)}$$

where, n_i is an unit vector. Substitute into equation 5:

$$\bar{q}=\frac{1}{V}\sum_{pipes}\frac{1}{12\mu} a^3 \Delta P n_i \quad \text{--- (eqn.7)}$$

The pressure difference between two points separated by vector distance Ln_j is:

$$\Delta P = Ln_j \frac{\partial P}{\partial x_j} \quad \text{--- (eqn.8)}$$

Substituting in equation 7:

$$\bar{q}=\frac{1}{V}\frac{\partial P}{\partial x_j}\sum_{pipes}\frac{1}{12\mu} a^3 L n_i n_j \quad \text{--- (eqn.9)}$$

Comparing with equation 1, the permeability can be expressed as:

$$k_{ij}=\frac{1}{V}\sum_{pipes}\frac{1}{12} a^3 L n_i n_j \quad \text{--- (eqn.10)}$$

In the special case of an isotropic medium where, $n_i = n_j$, leading to $n_i n_j = 1$

$$\bar{k} \equiv \frac{1}{2}k_{ij}=\frac{1}{24V}\sum_{pipes} a^3 L \quad \text{--- (eqn.11)}$$

We can calculate the total volume of the assembly by taking the sum of particle volumes and dividing by $1\text{-}n$, where n is the mean porosity. Equation 11, then, becomes:

$$\bar{k}=\frac{1\text{-}n}{24\pi\sum_{balls} R^2}\sum_{pipes} L a^3 \quad \text{--- (eqn.12)}$$

If we assume that all apertures are the same (this is only valid for a statistically uniform assembly) then we can estimate the aperture by:

$$a=\sqrt[3]{\frac{24\bar{k}\pi\sum_{balls} R^2}{(1\text{-}n)\sum_{pipes} L}} \quad \text{--- (eqn.13)}$$

In this way, the residual aperture required for a given permeability can be estimated. Figure 2 presents how the residual aperture is assigned to a contact. Aperture is simply the distance of

separation between two particles. But the actual aperture assigned to equation 1 is different. If the two particles are experiencing just touching without any compression or tension, then the distance of separation is geometrically zero. But we assume that non-zero aperture actually exists at the contact. We call this 'residual' aperture and it is expressed by equation 13. When the two touching particles are compressed, i.e. when they overlap, then the aperture at the contact shows non-linear decrease as expressed by equation 2. However, when there exists tensile force at the contact, i.e. in case of separation, residual aperture is assigned as an actual aperture used for calculation of volumetric fluid flow through the pipe. We use this assumption because when the aperture gets bigger and bigger, it results in very large flow rate which leads to very small calculation time step and consequently leads to instability of numerical calculation which should be avoided. When the tensile contact force further increases, then the contact experiences bond breakage. Even in this case, the residual aperture is still used for volumetric fluid flow calculation.

3. BIAXIAL COMPRESSION SIMULATION

The solid particle pore fluid coupling scheme is applied to a series of biaxial compression simulation. Strength variations of the model under pore fluid pressure and various confining pressure are examined and compared to the experimental findings from various laboratory tests on geo-materials. Also, moment tensor analysis of bond breakages is done and the seismic characteristics of cracking are analyzed mostly focusing on b-value variations.

3.1 Strength variation

The macroproperties presented in Figure 3 are calculated from the obtained peak strength data at confining pressures ranging from 2 MPa to 50 MPa. The results are presented by Mohr circles. Macroproperties to be compared are: peak strength envelop assuming that the model is an equivalent Mohr-Coulomb material with internal friction angle and cohesion. The relationships between peak strength and confining pressure under 0 and 5 MPa pore fluid pressures are shown in Figure 3. Pore fluid pressure being zero denotes the results of biaxial compression simulations without the coupling scheme. At the same confining pressure the rock models with pore fluid pressure have lower peak strength than those with 0 MPa pore fluid pressure. This is supported by the theory of effective stress, where the Mohr circle is translated leftward by an amount equal to the fluid pressure. The influence of pore fluid pressure on the strength can be analyzed in two ways. First, the effective stress of the porous medium drops because of pore fluid pressure.

Secondly, according to CT real-time testing of water on crack growth in fracutred rock mass by Li et al. [6], the water accelerates failure of rock mass by enhancing coalescence of microcracks, and results in decrement of rock strength. Assuming that the models are equivalent to Mohr-Coulomb materials, macroproperties of the models under 5 MPa pore fluid pressure are obtained. Result indicates that the angle of internal friction angle is much reduced by the presence of pore fluid pressure. However, cohesion does not show as much decrease as the internal friction angle.

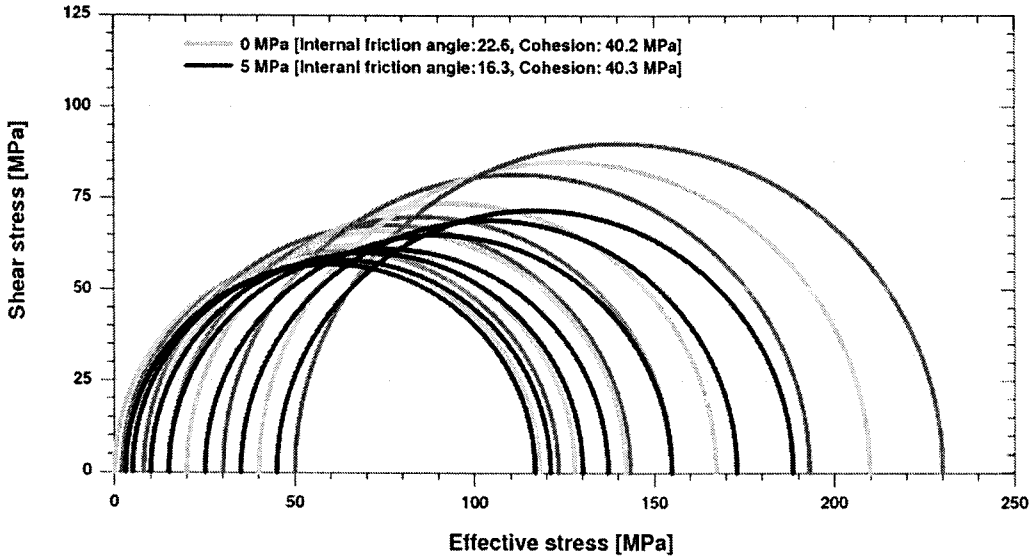

Fig. 3 Mohr circles for granite models in hydro-mechanical coupled biaxial compression simulations.

3.2 b-value variation

Seismic magnitudes of crack sources are also monitored throughout the loading. A typical plot of frequency-magnitude relation is presented in Figure 4a. Magnitude of the crack sources are calculated using the technique developed by Hazzard and Young [7]. It simulates seismicity in brittle rock under stress using PFC where the rock is represented by thousands of individual particles bonded together at points of contact. Seismicity results when bonds break under high local stresses and stored strain energy is released as kinetic energy. Details of the technique and its engineering applications are provided in the references [5,7,8].

There has been an interesting observation in the studies of uniaxial and triaxial compression tests on rock materials that a close analogy exists between acoustic emission produced from materials under brittle failure at the laboratory scale and seismic waves caused due to earthquakes.

This fact has motivated non-destructive testing to refine the acoustic emission technique such that it can serve as a tool for monitoring and also to forewarn the impending failure in engineering materials including rocks at several scales and earthquakes. Among various parameters, the most significant one is the b-value which is derived from the amplitude distribution data of acoustic emission following the method used in seismology. The b-value is defined as the log-linear slope of the frequency-magnitude distribution which is found to obey the Gutenberg-Richter relation, i.e. logN=a+bM [9], where N is the number of events which occurred of magnitude M, and a and b constants.

The cumulative number of crack events is plotted against magnitude in Figure 4b for those cases when the confining pressure is 40 MPa with 0, 1, 3, 5 MPa pore fluid pressure. Linear regression fit is used on the data within the magnitude range between -4.50 and -4.75. Slopes of the linear part of the curves correspond to b-values. According to Rao and Prasanna Lakshmi [10], a high b-value arises due to a large number of small acoustic emission hits representing new crack formation and slow crack growth, whereas a low b-value indicates faster or unstable crack growth accompanied by relatively high amplitude acoustic emission in larger numbers. Figure shows a trend that b-value decreases as the internal pore fluid pressure increases. This can be explained as that when the pore fluids are pressurized, they will act as wedges. It means that when the rock sample is loaded, volume contraction of the pore fluids is less than that of bulk rock so that pore fluids produce new stress concentration and enhance crack development. Because of the newly developed cracks and coalescences of those cracks into macro-fractures, unstable crack growth will be enhanced marked by relatively high amplitude acoustic emission which will eventually leads to low b-values. This is also supported by Scholz's experimental observations where he monitored the frequency-magnitude relations of Westerly granite under uniaxial and triaxial compression. It was found that the frequency-magnitude relation for events which accompanied frictional sliding and deformation of a ductile rock was found to have a much higher b-value than that observed in brittle rock [11]. As the figure shows, b-value decreases as the pore fluid pressure increases which demonstrates that the increasing pore fluid pressure enhances the brittleness of failure. This supports the statements above by Rao and Prasanna Lakshmi that pore fluid pressure enhances faster and unstable crack growth. Differences of b-values for different sample conditions (dry and wet) are experimentally verified by Zang et al. [12]. They performed uniaxial compression tests on dry and wet Flechtingen sandstones and calculated b-values from AE pulse statistics. It was found that b-value in the dry core sample was about 4.2 whereas that of wet core sample was 2.2, which also provides basis for explaining the results presented above and eventually leads to conclusion that the developed hydro-mechanical coupling scheme provides reasonable basis for rock modeling under pore fluid pressure. Also, Li et al. developed a nonlinear

dynamic computer model to simulate and analyze the features of the seismicity disturbance by pore fluid [13]. From the comparison of the seismicity of the dry and wet models, they found that there is a prominent difference. It showed that if there is fluid in the model and the fluid migrates with fluid diffusion equation, the frequency of shocks which takes place in the system and the energy accumulation rate are higher. The calculated b-values in the wet models showed that they are lower than those in the dry system.

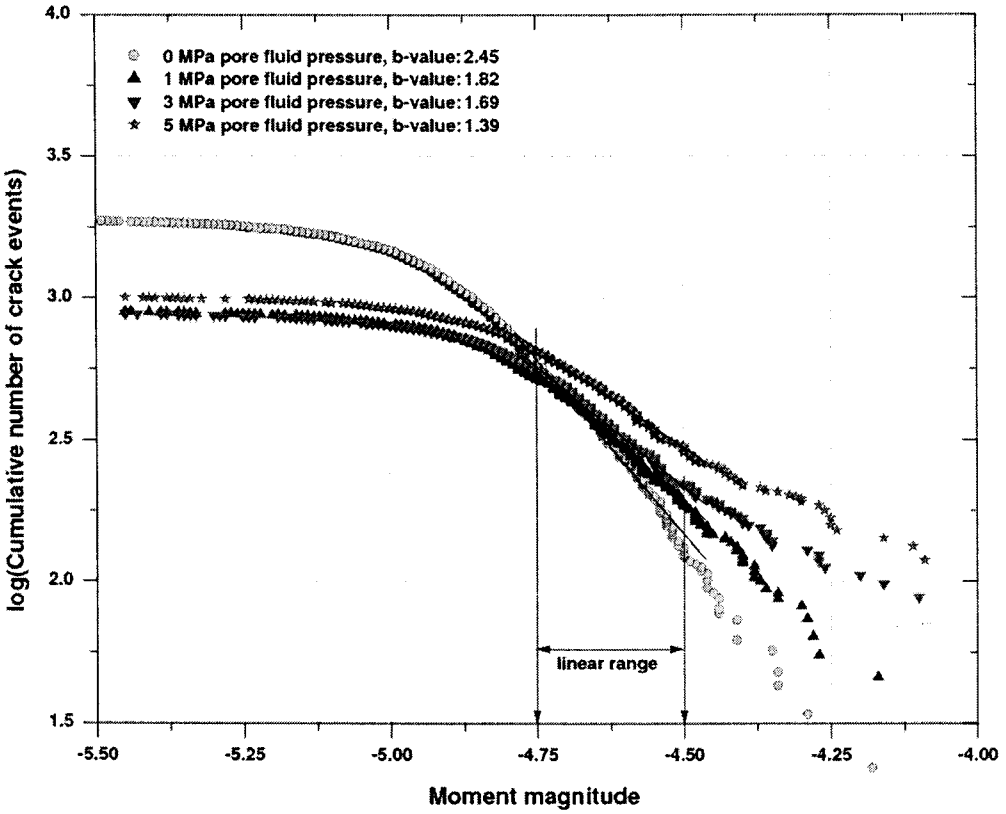

Fig. 4 Frequency-magnitude relations of seismic sources in granite models subjected to 40 MPa confining pressure under various levels of pore fluid pressures.

4. CONCLUSIONS

There have been several models developed with the aim of understanding the microscopic dissipative processes that occur during rock fracturing and their relation to the macroscopic progressive mechanical breakdown of rock in compression and associated fluid flow behavior. In this chapter, problems of bonded particle model based pore fluid solid particle coupling have been

discussed. The results obtained are in good agreement with what is known from corresponding experiments with geo-materials. Especially the simulation of biaxial compression test suggests that fluid plays a crucial role on the strength, seismic characteristics, and fracturing of rock sustaining internal pore fluid pressure.

The following conclusions are drawn:

1) Modeling of coupled interaction between pore fluids and solid particles is formulated. This new hydro-mechanical coupling scheme is applied to biaxial compression simulations. The introduction of pore fluid plays a crucial role for the strength, deformation and fracturing characteristics in rock models. Mechanical effect of pore fluid on strength has been well reproduced both in biaxial compression simulations.

2) Seismic characteristics of cracking are monitored and analyzed. Calculated b-values in rock models exhibited similar tendency as is observed in seismology. Introduction of pore fluids accelerates the failure process of the models, hence results in low b-value, which means faster and unstable crack growth are accompanied by large number of relatively high amplitude AE. Dependency of b-values on pore fluid pressure is well captured.

3) It is conclusive that the model predictions of mechanical and seismic behavior of rocks using the developed hydro-mechanical coupling scheme captures most of the experimental observations, especially the confining pressure effect and pore pressure effect of rock specimens in biaxial compression.

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