HYDRO-MECHANICAL COUPLING OF SHEAR-INDUCED ROCK FRACTURING BY BONDED PARTICLE MODELING

A THESIS SUMMARY

BY

JEOUNGSEOK YOON
CONTENTS

ABSTRACT 3
1. INTRODUCTION 5
2. A NEW METHOD FOR MICROPARAMETER DETERMINATION 6
  2.1 Bonded particle model and microparameters 7
  2.2 Methodologies 7
  2.3 Plackett-Burman design 8
  2.4 Central Composite Design 12
  2.5 Optimization 15
  2.6 Verification of solution 17
  2.7 Conclusions 20
3. HYDRO-MECHANICAL COUPLING IN BONDED PARTICLE MODEL 22
  3.1 Coupling of solid particles and pore fluids 23
    3.1.1 Generation of pore fluid network 23
    3.1.2 Formulation of fluid flow 23
    3.1.3 Aperture calculation 24
  3.2 Verification problems 27
    3.2.1 Pore fluid permeation 27
    3.2.2 Biaxial compression simulation 28
  3.3 Conclusions 32
4. NUMERICAL AND EXPERIMENTAL STUDIES ON CONFINED SHEAR-INDUCED FRACTURING OF ROCKS 34
  4.1 Bonded particle modeling of PTS test 34
  4.2 Simulation results – Effect of presence of pore fluid 36
  4.3 Laboratory PTS test 41
  4.4 Experimental results – Effect of saturation 42
    4.4.1 Effect of saturation on strength and deformation 43
    4.4.2 Effect of loading rate on strength in saturated condition 44
    4.4.3 Fracture inspection 45
  4.5 Conclusions 49
5. SUMMARY 50
SELECTED REFERENCES 52
ABSTRACT

Presence of fluid or fluid pressure exerts a significant influence on rock strength and deformation and it occurs from grain-scale to lithospheric-scale. This has led to a necessity of understanding the hydro-mechanical coupled processes. And with the appearance of mature computing methods and hardwares becoming available, development of an appropriate numerical tool which can handle the complexity of hydro-mechanical coupled behavior of rock materials has been recognized as one of the major tasks in rock engineering field.

With this background, the thesis presents a numerical technique that can simulate the hydro-mechanical coupling in bonded particle model using the commercially available Particle Flow Code 2D (PFC2D). The thesis starts with a suggestion of a method that can simplify the process of microparameter determination for model generation. The question of how to properly choose the microparameters has interested many researchers that the process of microparameter determination can be subjective and time consuming. The new method incorporates Design of Experiment and optimization. Microparameters obtained by the method were proved to give good agreements between the results from laboratory uniaxial compression tests with those from simulations. Reliability of the new method is later, again, verified by applying it to simulation of asymmetric triaxial compression test. Comparison of the results from the laboratory tests with those from simulations in which the new method was applied to model generation showed fair agreements by which the reliability of the new method for microparameter determination was proved.

Once the problem of microparameter determination is solved, then, the thesis continues with a new method of hydro-mechanical coupling based on the former algorithms by Cundall and Hazzard. It was later applied to biaxial compression simulations and variations of strength, fracturing and failure patterns, and b-value under pore fluid pressure were compared with the experimental results on rock materials from various reference data which were proved to be consistent. Using the seismic monitoring technique proposed by Hazzard, in the thesis, it was proved that introduction of pore fluids accelerates the failure process of models; hence results in b-value decrease which means that faster and unstable crack growth are accompanied. Dependency of b-value in simulations and experimental observations from various reference data were consistent.
Then the thesis continues with shear fracturing of rocks. Confined shear fracturing is technically induced by Punch Through Shear (PTS) test. Series of laboratory PTS test were conducted on the dry and saturated granite in order to examine the effect of saturation on strength, fracturing and failure patterns under various levels of confining pressure and loading rates. The laboratory PTS test was reproduced by bonded particle modeling where the new hydro-mechanical coupling scheme was adopted to simulate the saturated granite. Comparisons between the simulation results and those from laboratory PTS tests showed good agreements which led to a conclusion that the developed hydro-mechanical coupling was successful in simulating the shear-induced fracturing behaviors of rocks under the presence of pore fluid.

Laboratory experiments and numerical simulations were focused on the examination of confined shear-induced fracturing and failure in saturated rocks, so that in situ settings of subsurface reservoir and underground caverns could be reflected, of which pre-existing fractures in rock mass are exposed to confined shear loading under saturated conditions. The correlation of the numerical simulations results to laboratory observations will allow for the improved assessment of hydro-mechanically coupled processes of geo-materials.
1. INTRODUCTION

Summary of the thesis consists of three chapters which are distinguished as follows.

Chapter 2 – A new method for microparameter determination

Chapter deals with a development process of a new method for microparameter determination in model generation using Design of Experiment and optimization. Validity of the new method is tested by comparing uniaxial compression simulation results with laboratory test data, which proved to be reliable.

Chapter 3 – Hydro-mechanical coupling in bonded particle model

Hydro-mechanical coupling in bonded particle model is developed based on the former fluid solid interaction algorithms proposed by Cundall and Hazzard. It is applied to biaxial compression simulation and variations of strength, deformation, and seismic characteristics under the presence of pore fluid pressure are compared with data from various experiments. Comparisons are examined to prove the reliability of the hydro-mechanical coupling scheme.

Chapter 4 – Numerical and experimental studies on confined shear-induced fracturing of rocks

Shear fracture is induced by PTS test on dry and saturated granite. The results of PTS tests, e.g. strength, dependence of $K_{IC}$ on the presence of pore fluid, confining pressure, loading rate, and fracturing patterns, etc. are compared with those from simulations.

Finally, Chapter 5 summarizes the major results obtained in this study.
2. A NEW METHOD FOR MICROPARAMETER DETERMINATION

Discrete Element Method (DEM) simulates the mechanical behavior of rock by idealizing the system as a collection of structural units such as springs, beams, or separate particles bonded together at their contact points and it utilizes the breakage of individual structural units or bonds to directly represent damage. The PFC2D is a type of DEM, which is commercially available and widely used to solve geo-mechanical problems.

All numerical simulations by PFC2D require proper selection of microparameters by means of calibration process in which the responses of the numerical model are compared directly to the observed responses of the physical material. This has been done so far by “trial and error” which requires a few times of repetitive work. There have been a few attempts to improve and simplify the calibration procedure and a recent suggestion for PFC2D model calibration is provided by Jong and Lee (2006) in which they suggested a straight-forward way of calculating the microparameters for uniaxial compression simulation.

The objective of this chapter is to develop a new and better method that calculates the proper microparameters for model generation in uniaxial compression simulation. With this approach, a set of microparameters is obtained by which the generated model closely reproduces physical properties of the target rock material; Uniaxial Compressive Strength (UCS), Young’s modulus, and Poisson’s ratio.

New approach starts with the Design of Experiment. The Plackett-Burman design method is used to determine the microparameters having the largest impacts on macroscopic responses. Then, non-linear relations between the selected microparameters and macroscopic responses are estimated using the Central Composite Design. Optimization method is then used to calculate an optimum set of microparameters which provides the best quantitative and qualitative agreements between the responses of a bonded particle models and those of tested rock materials. Once the optimum microparameters are obtained, then they are used to generate a contact bond model. Uniaxial compression simulation is then carried out on the generated model and the results; strength, elastic constants and crack distribution, are compared with the results of a laboratory test for verifying the adequacy of the solution and also the applicability of the new method.
2.1 Bonded particle model and microparameters

In PFC2D simulation, rock material is represented as an assembly of circular disks bonded together at their contact points and confined by walls. The particles are bonded together at their contacts to simulate a competent rock. The contact bonds are assigned with specified tensile and shear strength so that resistance to tension and shear exists at the contacts until the force at the contact exceeds the strength of the bond. Overall mechanism of the system is well documented in the references (Itasca CG, 2004; Potyondy & Cundall, 2004). In order to generate a contact bond model using the biaxial compression simulations routine provided in the reference, the following microparameters should be defined and assumed to be the complete set for generating a contact bond model:

- Ball-to-ball Contact Modulus: BCM
- Stiffness ratio, $\frac{K_N}{K_S}$
- Ball Friction coefficient: FRIC
- Contact Normal Bond Strength: NBS
- Contact Shear Bond Strength: SBS
- Ratio Of Standard Deviation to mean of bond strength: ROSD
- Minimum Ball Radius: BRAD

2.2 Methodologies

Design of Experiment (DOE) is defined as a structured, organized method for determining the relationship between factors affecting a process and the output of that process. Experimentalists change one or several process variables (factors or parameters) in order to observe the effect the changes have on one or several response variables. DOE begins with determining the objectives of an experiment and selecting the process variables for the study. In this study, process variables are referred to those listed seven microparameters and response variables are referred to the results of uniaxial compression simulations; UCS, Young’s modulus and Poisson’s ratio. Two DOE methods are applied to sensitivity analysis of microparameters of contact bond models. They are Plackett-Burman (PB) design and Central Composite Design (CCD). For screening purpose, the PB design method is adopted. This design allows reliable short listing of a small number of factors for further optimization and allows one to obtain unbiased estimates of linear effects of all the factors with maximum accuracy for a given number of observations, the accuracy being the same for all effects (Plackett & Burman, 1946; Krishnan et al., 1998). Response variables are expressed by linear combination of several independent process variables. However, in order to precisely estimate the responses, the experiment has to be designed to allow estimate of interaction and even quadratic effects of each independent process variable. For this purpose, the CCD is applied which is capable
of estimating interaction and quadratic effects.

The strategy adopted in optimization is that we try to get a set of microparameters for generating a contact bond model for which results of uniaxial compression simulations closely match those from testing of rock materials. Constraints are imposed which affect the computation of solution. Relations between microparameters are transformed into functional forms which are imposed on optimization process and those constraints affect the determination of solution. The problem is solved by non-linear constrained optimization programming using the Matlab optimization toolbox.

2.3 Plackett-Burman design

Table 2.1 lists the microparameters with their minus level (lower bound) and plus level (upper bound) and zero level which is an arithmetic mean of the two. The values of minus and plus levels for each microparameters should be defined based on their practical physical meanings. Caution must be exercised while setting the level differential, as a small differential may not show any effect and a large differential for a sensitive component can mask other components (Ahuja et al., 2004). Example of level assignments in application of two level full factorial design is presented in the reference (Starzec & Andersson, 2002).

Figure 2.1 shows relation between the UCS and microparameter NBS and SBS. From the linear relation and an assumption that UCS for hard rocks falls within a range between 70 and 250 MPa, -1 and +1 levels of NBS and SBS were assigned to 50 and 200 MPa, respectively. Figure 2.2 and Figure 2.3 show the relations between the BCM and Young’s modulus, and the KNKS and Poisson’s ratio, respectively. From the relations, -1 and +1 levels of the BCM and KNKS are obtained. Determination of the lower and upper bounds for the ROSD is more complicated and requires use of crack initiation stress thresholds for the test materials. Crack initiation stress thresholds are obtained by laboratory tests (Eberhardt, 1998; Eberhardt et al., 1999; Yoon, 2002a) which is defined as the axial stress at which non-elastic dilation begins. Crack initiation stress in PFC simulation is defined as the axial stress at which there exists a specified fraction of total number of cracks existing in the model at the point where the peak strength has been obtained (Itasca CG, 2004; Potyondy & Cundall, 2004). The specified fraction is governed by a subroutine variable ‘pk_ci_fac’ and it was changed from 1% to 8% and the corresponding stress thresholds were computed (Figure 2.4). In this study, we focus on the overlapping encircled area at which the given lower and upper bounds for the ROSD are 0.24 and 0.40, respectively (Figure 2.4).

Particle friction coefficient is known to affect only post-peak response in contact bonded model (Potyondy & Cundall, 2004). Because, when a contact bond between the two touching particles
breaks, then slip model is activated and slip of the two particles are governed only by the particle friction coefficient (Itasca CG, 2004). However, it is not clear to what it should be calibrated, thus 0.50 is assigned to zero level for particle friction coefficient as a reasonable non-zero value. And for -1 and +1 level, ±50% offsets of the zero level value were assigned to each.

To look into the influence of model resolution on the responses, minimum particle radius (BRAD) is varied from 0.24 mm to 0.48 mm. The size distribution of the particles follows uniform distribution and the average particle diameter of the model generated by using a minimum particle radius of 0.24 mm and 0.48 mm are 0.64 mm and 1.28 mm, respectively.

Table 2.1 Microparameters and coded level for PB design.

<table>
<thead>
<tr>
<th>Microparameter (unit)</th>
<th>Levels (coded)</th>
<th>Coded to Uncoded</th>
</tr>
</thead>
<tbody>
<tr>
<td>BCM (GPa)</td>
<td>-1 70 100</td>
<td>uncoded = 30coded + 70</td>
</tr>
<tr>
<td>KNKS (---)</td>
<td>1.0 2.5 4.0</td>
<td>uncoded = 1.5coded + 2.5</td>
</tr>
<tr>
<td>FRIC (---)</td>
<td>0.25 0.50 0.75</td>
<td>uncoded = 0.25coded + 0.5</td>
</tr>
<tr>
<td>NBS (MPa)</td>
<td>50 125 200</td>
<td>uncoded = 75coded + 125</td>
</tr>
<tr>
<td>SBS (MPa)</td>
<td>50 125 200</td>
<td>uncoded = 75coded + 125</td>
</tr>
<tr>
<td>ROSD (---)</td>
<td>0.24 0.32 0.40</td>
<td>uncoded = 0.08coded + 0.32</td>
</tr>
<tr>
<td>BRAD (mm)</td>
<td>0.24 0.36 0.48</td>
<td>uncoded = 0.12coded + 0.36</td>
</tr>
</tbody>
</table>

The complete design matrix for PB screening design is shown in Table 2.2. Each factor settings, i.e. coded as -1 and +1, are transformed to uncoded values by transformation equations given in the last column of Table 2.1. These uncoded values of microparameters are used for generating contact bond models, one for the uniaxial compression test simulation (50 mm width, 100 mm height) and the other for the Brazilian tensile test simulation (50 mm diameter). Therefore, in total, 12 models are generated and UCS, Young’s modulus, Poisson’s ratio, and Brazilian tensile strength are calculated (Table 2.3).

Table 2.2 Complete design matrix for PB design.

<table>
<thead>
<tr>
<th>No.</th>
<th>BCM</th>
<th>KNKS</th>
<th>FRIC</th>
<th>NBS</th>
<th>SBS</th>
<th>ROSD</th>
<th>BRAD</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>-1</td>
<td>+1</td>
<td>+1</td>
<td>+1</td>
<td>-1</td>
<td>-1</td>
<td>-1</td>
</tr>
<tr>
<td>2</td>
<td>-1</td>
<td>-1</td>
<td>-1</td>
<td>+1</td>
<td>-1</td>
<td>-1</td>
<td>+1</td>
</tr>
<tr>
<td>3</td>
<td>+1</td>
<td>+1</td>
<td>-1</td>
<td>+1</td>
<td>-1</td>
<td>+1</td>
<td>+1</td>
</tr>
<tr>
<td>4</td>
<td>+1</td>
<td>-1</td>
<td>+1</td>
<td>-1</td>
<td>-1</td>
<td>+1</td>
<td>-1</td>
</tr>
<tr>
<td>5</td>
<td>+1</td>
<td>+1</td>
<td>+1</td>
<td>+1</td>
<td>+1</td>
<td>-1</td>
<td>-1</td>
</tr>
<tr>
<td>6</td>
<td>+1</td>
<td>-1</td>
<td>+1</td>
<td>+1</td>
<td>-1</td>
<td>+1</td>
<td>+1</td>
</tr>
<tr>
<td>7</td>
<td>+1</td>
<td>+1</td>
<td>+1</td>
<td>-1</td>
<td>-1</td>
<td>-1</td>
<td>+1</td>
</tr>
<tr>
<td>8</td>
<td>+1</td>
<td>+1</td>
<td>-1</td>
<td>-1</td>
<td>-1</td>
<td>+1</td>
<td>-1</td>
</tr>
<tr>
<td>9</td>
<td>+1</td>
<td>-1</td>
<td>-1</td>
<td>+1</td>
<td>-1</td>
<td>-1</td>
<td>+1</td>
</tr>
<tr>
<td>10</td>
<td>-1</td>
<td>+1</td>
<td>-1</td>
<td>+1</td>
<td>-1</td>
<td>+1</td>
<td>+1</td>
</tr>
<tr>
<td>11</td>
<td>-1</td>
<td>-1</td>
<td>+1</td>
<td>-1</td>
<td>-1</td>
<td>+1</td>
<td>-1</td>
</tr>
<tr>
<td>12</td>
<td>-1</td>
<td>-1</td>
<td>+1</td>
<td>-1</td>
<td>+1</td>
<td>+1</td>
<td>+1</td>
</tr>
</tbody>
</table>
Figure 2.1 Linear relation between the NBS and SBS and UCS. Typical values of UCS for hard rocks are assumed to fall within the encircled area.

Figure 2.2 Linear relation between the BCM and Young's modulus. Typical values of Young's modulus for hard rocks are assumed to fall within the encircled area.
Figure 2.3 Relation between the KNKS and Poisson’s ratio (modified from Itasca CG, 2004). Typical values of Poisson’s ratio for hard rocks are assumed to fall within the encircled area.

Figure 2.4 Relation between the ROSD and crack initiation stress. Crack initiation thresholds are taken from experimental findings (Eberhardt, 1998; Eberhardt et al., 1999; Yoon, 2002a).
Table 2.3 Results of uniaxial compression simulations on 12 models.

<table>
<thead>
<tr>
<th>No.</th>
<th>Y1 UCS [MPa]</th>
<th>Y2 Young's modulus [GPa]</th>
<th>Y3 Poisson's ratio</th>
<th>Y4 Brazilian tensile strength [MPa]</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>86.56</td>
<td>23.16</td>
<td>0.234</td>
<td>22.02</td>
</tr>
<tr>
<td>2</td>
<td>58.96</td>
<td>33.75</td>
<td>0.122</td>
<td>15.49</td>
</tr>
<tr>
<td>3</td>
<td>77.98</td>
<td>22.40</td>
<td>0.266</td>
<td>19.45</td>
</tr>
<tr>
<td>4</td>
<td>91.47</td>
<td>86.92</td>
<td>0.100</td>
<td>18.37</td>
</tr>
<tr>
<td>5</td>
<td>196.27</td>
<td>55.37</td>
<td>0.273</td>
<td>51.55</td>
</tr>
<tr>
<td>6</td>
<td>225.02</td>
<td>87.01</td>
<td>0.097</td>
<td>50.26</td>
</tr>
<tr>
<td>7</td>
<td>58.23</td>
<td>55.70</td>
<td>0.265</td>
<td>12.36</td>
</tr>
<tr>
<td>8</td>
<td>45.59</td>
<td>55.81</td>
<td>0.268</td>
<td>9.55</td>
</tr>
<tr>
<td>9</td>
<td>45.74</td>
<td>83.18</td>
<td>0.113</td>
<td>18.93</td>
</tr>
<tr>
<td>10</td>
<td>199.81</td>
<td>23.00</td>
<td>0.247</td>
<td>38.56</td>
</tr>
<tr>
<td>11</td>
<td>46.67</td>
<td>33.64</td>
<td>0.103</td>
<td>10.12</td>
</tr>
<tr>
<td>12</td>
<td>86.37</td>
<td>33.62</td>
<td>0.130</td>
<td>16.70</td>
</tr>
<tr>
<td>Range</td>
<td>46-225</td>
<td>22-87</td>
<td>0.10-0.27</td>
<td>9.6-51.6</td>
</tr>
</tbody>
</table>

Table 2.4 lists the coefficients of the microparameters and those underlined are the coefficients of the microparameters that have significant effects on the response. The absolute value of the coefficient determines its relative strength. The higher the value, the greater is the effect on the response. The sign of the coefficient determines which factor setting results in a higher response measurement. For example, in case of Y2 (Young's modulus), factor KNKS has a negative coefficient, i.e. -10.30. This means that if the factor setting of KNKS is shifted from -1 to +1 level, i.e. increasing, then this results in decrease of the response Y2. Coefficients are used to construct linear regression fits, which will be used as linear equality and inequality constraints in the optimization. Linear fits for each response are constructed as follows.

\[ Y1 = 101.56 + 8.83 \text{BCM} + 9.18 \text{KNKS} + 14.96 \text{FRIC} + 33.84 \text{NBS} + 44.60 \text{SBS} + 44.60 \text{ROSD} - 14.30 \text{BRAD} \]  
\[ Y2 = 49.54 + 21.28 \text{BCM} - 10.30 \text{KNKS} + 1.52 \text{FRIC} + 2.00 \text{NBS} + 2.10 \text{SBS} - 2.20 \text{ROSD} - 2.20 \text{BRAD} \]  
\[ Y3 = 0.1848 + 0.0012 \text{BCM} + 0.0740 \text{KNKS} - 0.0012 \text{FRIC} - 0.0038 \text{NBS} - 0.0006 \text{SBS} - 0.0042 \text{ROSD} + 0.0100 \text{BRAD} \]  
\[ Y4 = 23.613 + 3.223 \text{BCM} + 1.968 \text{KNKS} + 3.555 \text{FRIC} + 9.188 \text{NBS} + 8.868 \text{SBS} + 0.622 \text{ROSD} - 1.200 \text{BRAD} \]

2.4 Central Composite Design

Once the two microparameters having the biggest impacts are screened out of the original seven, then the responses are further estimated. A complete description of the response might require a quadratic model. These are the full models, with all possible combinations of terms considered. One of the methods used to predict quadratic curvature of the response is CCD. It contains an imbedded factorial or fractional factorial design with center points that are augmented with a group of ‘star points’ that allows estimation of curvature (Table 2.5). If the distance from the center of the design space to a factorial point is ±1 unit for each factor, the distance from the center of the
design space to a star point is ± \( \alpha \). In this case, there are two factors with two levels, therefore the number of factorial runs is 4, which results in \( \alpha = \sqrt{2} \).

Design matrices and the results of the CCD analysis are presented in Table 2.6. For the response Y5 (UCS), model are generated using the factor setting of NBS and SBS listed in the table. Rests of the microparameters are set to zero level listed in Table 2.1. For the responses Y5 (UCS) and Y8 (Brazilian tensile strength), the two most significant microparameters selected are NBS and SBS. For the response Y6 (Young's modulus), microparameters BCM and KNKS are selected and for the response Y7 (Poisson's ratio), KNKS and BRAD are selected. Table 2.7 lists the coefficients obtained from the CCD analyses which are used to construct the regression fits for each response. They contain coefficients for the two-factor-interaction effects and for the squared effects of single factors. The following are constructed using the coefficients in Table 2.7 and are used as nonlinear inequality constraints in optimization.

\[
\begin{align*}
Y_5 &= 128.79 + 41.86 \text{NBS} + 43.97 \text{SBS} - 14.49 \text{NBS}^2 - 16.66 \text{SBS}^2 + 30.42 \text{NBS} \cdot \text{SBS} \quad \text{---(eqn5)} \\
Y_6 &= 45.92 + 20.17 \text{BCM} - 11.31 \text{KNKS} - 0.11 \text{BCM}^2 + 3.93 \text{KNKS}^2 - 4.45 \text{BCM} \cdot \text{KNKS} \quad \text{---(eqn6)} \\
Y_7 &= 0.194 + 0.078 \text{KNKS} + 0.006 \text{BRAD} - 0.025 \text{KNKS}^2 + 0.001 \text{BRAD}^2 - 0.006 \text{KNKS} \cdot \text{BRAD} \quad \text{---(eqn7)} \\
Y_8 &= 30.29 + 10.28 \text{NBS} + 10.59 \text{SBS} - 3.84 \text{NBS}^2 - 3.32 \text{SBS}^2 + 6.42 \text{NBS} \cdot \text{SBS} \quad \text{---(eqn8)}
\end{align*}
\]

Table 2.5 Complete design matrix for CCD.

<table>
<thead>
<tr>
<th>Point type</th>
<th>Fac. 1</th>
<th>Fac. 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Corner (1)</td>
<td>-1</td>
<td>+1</td>
</tr>
<tr>
<td>Corner (2)</td>
<td>+1</td>
<td>+1</td>
</tr>
<tr>
<td>Corner (3)</td>
<td>+1</td>
<td>-1</td>
</tr>
<tr>
<td>Corner (4)</td>
<td>-1</td>
<td>-1</td>
</tr>
<tr>
<td>Star (a)</td>
<td>0</td>
<td>+ ( \sqrt{2} )</td>
</tr>
<tr>
<td>Star (b)</td>
<td>+ ( \sqrt{2} )</td>
<td>0</td>
</tr>
<tr>
<td>Star (c)</td>
<td>0</td>
<td>- ( \sqrt{2} )</td>
</tr>
<tr>
<td>Star (d)</td>
<td>- ( \sqrt{2} )</td>
<td>0</td>
</tr>
<tr>
<td>Center (i)</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Center (ii)</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Center (iii)</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Center (iv)</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Center (v)</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>
Table 2.4 Results of PB design.

<table>
<thead>
<tr>
<th>Factors</th>
<th>Y1 UCS</th>
<th>Y2 Young's modulus</th>
<th>Y3 Poisson's ratio</th>
<th>Y4 Brazilian tensile strength</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Coef(^a)</td>
<td>p(^b)</td>
<td>Order</td>
<td>Coef</td>
</tr>
<tr>
<td>Constant</td>
<td>101.56</td>
<td>0.000</td>
<td>-</td>
<td>49.54</td>
</tr>
<tr>
<td>BCM</td>
<td>8.83</td>
<td>0.340</td>
<td>6</td>
<td>21.28</td>
</tr>
<tr>
<td>KNKS</td>
<td>9.18</td>
<td>0.323</td>
<td>5</td>
<td>-10.30</td>
</tr>
<tr>
<td>FRIC</td>
<td>14.96</td>
<td>0.141</td>
<td>3</td>
<td>-1.31</td>
</tr>
<tr>
<td>NBS</td>
<td>33.84</td>
<td>0.014</td>
<td>2</td>
<td>1.52</td>
</tr>
<tr>
<td>SBS</td>
<td>44.60</td>
<td>0.005</td>
<td>1</td>
<td>2.00</td>
</tr>
<tr>
<td>ROSD</td>
<td>1.85</td>
<td>0.832</td>
<td>7</td>
<td>-2.10</td>
</tr>
<tr>
<td>BRAD</td>
<td>-14.30</td>
<td>0.155</td>
<td>4</td>
<td>-2.20</td>
</tr>
</tbody>
</table>

\(^a\) ‘Coeff’ defines relative strength of influence of a factor on a response and is used to construct linear regression fit.

\(^b\) ‘p’ determines whether the influence of the microparameter on the response is significant or not. If the p-value is less than or equal to 0.05, which is a commonly used level of significance, the factor is significant.
Table 2.6 Design matrices used in CCD and the results of uniaxial compression simulations on 13 models.

<table>
<thead>
<tr>
<th>No.</th>
<th>NBS</th>
<th>SBS</th>
<th>Y5</th>
<th>Y8</th>
<th>BCM</th>
<th>KNKS</th>
<th>Y6</th>
<th>KNKS</th>
<th>BRAD</th>
<th>Y7</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>-√2</td>
<td>0</td>
<td>32.81</td>
<td>6.58</td>
<td>0</td>
<td>0</td>
<td>45.92</td>
<td>√2</td>
<td>0</td>
<td>0.253</td>
</tr>
<tr>
<td>2</td>
<td>-1</td>
<td>1</td>
<td>75.04</td>
<td>16.48</td>
<td>0</td>
<td>√2</td>
<td>36.79</td>
<td>0</td>
<td>0</td>
<td>0.194</td>
</tr>
<tr>
<td>3</td>
<td>-1</td>
<td>-1</td>
<td>50.39</td>
<td>11.22</td>
<td>0</td>
<td>0</td>
<td>45.92</td>
<td>-1</td>
<td>1</td>
<td>0.114</td>
</tr>
<tr>
<td>4</td>
<td>1</td>
<td>-1</td>
<td>69.08</td>
<td>16.68</td>
<td>0</td>
<td>0</td>
<td>45.92</td>
<td>0</td>
<td>0</td>
<td>0.194</td>
</tr>
<tr>
<td>5</td>
<td>1</td>
<td>1</td>
<td>215.42</td>
<td>47.63</td>
<td>-1</td>
<td>1</td>
<td>22.48</td>
<td>-√2</td>
<td>0</td>
<td>0.019</td>
</tr>
<tr>
<td>6</td>
<td>0</td>
<td>0</td>
<td>128.79</td>
<td>30.29</td>
<td>1</td>
<td>1</td>
<td>55.78</td>
<td>-1</td>
<td>-1</td>
<td>0.093</td>
</tr>
<tr>
<td>7</td>
<td>0</td>
<td>0</td>
<td>128.79</td>
<td>30.29</td>
<td>√2</td>
<td>0</td>
<td>18.55</td>
<td>0</td>
<td>√2</td>
<td>0.178</td>
</tr>
<tr>
<td>8</td>
<td>0</td>
<td>0</td>
<td>128.79</td>
<td>30.29</td>
<td>0</td>
<td>-√2</td>
<td>70.92</td>
<td>0</td>
<td>√2</td>
<td>0.202</td>
</tr>
<tr>
<td>9</td>
<td>0</td>
<td>0</td>
<td>128.79</td>
<td>30.29</td>
<td>0</td>
<td>0</td>
<td>45.92</td>
<td>0</td>
<td>0</td>
<td>0.194</td>
</tr>
<tr>
<td>10</td>
<td>0</td>
<td>0</td>
<td>128.79</td>
<td>30.29</td>
<td>√2</td>
<td>0</td>
<td>72.98</td>
<td>1</td>
<td>1</td>
<td>0.250</td>
</tr>
<tr>
<td>11</td>
<td>√2</td>
<td>0</td>
<td>157.12</td>
<td>38.87</td>
<td>0</td>
<td>0</td>
<td>45.92</td>
<td>0</td>
<td>0</td>
<td>0.194</td>
</tr>
<tr>
<td>12</td>
<td>0</td>
<td>√2</td>
<td>154.54</td>
<td>40.89</td>
<td>-1</td>
<td>-1</td>
<td>34.68</td>
<td>0</td>
<td>0</td>
<td>0.194</td>
</tr>
<tr>
<td>13</td>
<td>0</td>
<td>-√2</td>
<td>26.69</td>
<td>6.59</td>
<td>1</td>
<td>-1</td>
<td>85.79</td>
<td>1</td>
<td>-1</td>
<td>0.252</td>
</tr>
</tbody>
</table>

Table 2.7 Results of CCD.

<table>
<thead>
<tr>
<th>Terms</th>
<th>Y5</th>
<th>Coeff</th>
<th>Terms</th>
<th>Y6</th>
<th>Coeff</th>
<th>Terms</th>
<th>Y7</th>
<th>Coeff</th>
</tr>
</thead>
<tbody>
<tr>
<td>Constant</td>
<td>128.79</td>
<td>30.29</td>
<td>Constant</td>
<td>45.92</td>
<td></td>
<td>Constant</td>
<td>0.194</td>
<td></td>
</tr>
<tr>
<td>NBS</td>
<td>41.86</td>
<td>10.28</td>
<td>BCM</td>
<td>20.17</td>
<td></td>
<td>KNKS</td>
<td>0.078</td>
<td></td>
</tr>
<tr>
<td>SBS</td>
<td>43.97</td>
<td>10.59</td>
<td>KNKS</td>
<td>-11.31</td>
<td></td>
<td>BRAD</td>
<td>0.006</td>
<td></td>
</tr>
<tr>
<td>NBS²</td>
<td>-14.49</td>
<td>-3.84</td>
<td>BCM²</td>
<td>-0.11</td>
<td></td>
<td>KNKS²</td>
<td>-0.025</td>
<td></td>
</tr>
<tr>
<td>SBS²</td>
<td>-16.66</td>
<td>-3.32</td>
<td>KNKS²</td>
<td>3.93</td>
<td></td>
<td>BRAD²</td>
<td>0.001</td>
<td></td>
</tr>
<tr>
<td>NBS-SBS</td>
<td>30.42</td>
<td>6.42</td>
<td>BCM-KNKS</td>
<td>-4.45</td>
<td></td>
<td>KNKS-BRAD</td>
<td>-0.006</td>
<td></td>
</tr>
</tbody>
</table>

2.5 Optimization

Optimization method is used to calculate the microparameters which give the closest match between the results from a laboratory test and those from a simulation. We are interested in matching UCS, Young’s modulus, and Poisson’s ratio. In order to formulate an optimization problem it is required to express the problem including its objective and circumstances in mathematical form. The objective is to make the absolute value of the difference between the two UCS, one from laboratory test and the other from simulation close to zero. It is rewritten into a functional form as follows.

Objective function, \( f = \text{Minimize} |\text{Simulation UCS} - \text{Laboratory test UCS}| \)

To construct the objective function, the ‘Simulation UCS’ is replaced by regression fit obtained by the CCD analysis, 2nd order polynomial regression fit. Several constraints are imposed on the optimization problem in order to restrict the solution within reasonable ranges and to give it a physical basis. There are four types of constraints and their definitions are summarized as follows.

Type 1 – Linear equality constraints

- UCS of a model should be close to (or equal, if possible) that of a tested rock
specimen. Equation (1) is used to formulate this constraint.

- Young's modulus of a model should be close to (or equal, if possible) that of a tested rock specimen. Equation (2) is used to formulate this constraint.

- Poisson's ratio of a model should be close to (or equal, if possible) that of a tested rock sample. Equation (3) is used to formulate this constraint.

Type 2 – Linear inequality constraints

- Ratio of UCS to Brazilian tensile strength of a model should be between 3 and 10. The UCS of a model and its Brazilian tensile strength are represented by Equation (1) and (4), respectively.

- Ratio of SBS to NBS should be between 1 and 3. It is assumed that NBS and SBS are physically related to mode I and mode II fracture toughness (KIC, KIIC). Ratios of KIIC to KIC are in fair agreement with the ratio of 1-3 commonly referred in literature (Al-Shayea et al., 2000; Ingraffea, 1981; Rao et al., 2003; Backers, 2005).

Type 3 – Nonlinear inequality constraints

- Ratio of UCS to Brazilian tensile strength of a model should be between 3 and 10. The UCS of a model and its Brazilian tensile strength are represented by equation (5) and (8), respectively. The only difference from the linear inequality constraint is that Equation (5) and (8) are functions of only NBS and SBS and they involve interaction and squared effects of NBS and SBS.

Type 4 – Side constraints

- All the microparameters should be between their prescribed lower (-1) and upper (+1) limits. This constraint regulates the calculation of the optimization problem so that the solution stays within the feasible region.

The optimization problem is solved by using function fmincon provided in Matlab optimization toolbox (version 2.0). A set of microparameters is called optimum because it is supposed to satisfy the objective as well as the imposed constraints. Set of microparameters is computed at each computation step, and the optimization solver keeps track of values of the objective function and searches for the optimum solution and checks whether the imposed constraints are satisfied.
2.6 Verification of solution

Final step is to check the adequacy of the optimum solution. The optimization process is supposed to provide the best microparameters for model generation which give the closest match between the results of laboratory test and those from a simulation on the generated models. The adequacy and optimality of the solution can be checked simply by comparing the numbers of UCS, Young’s modulus, Poisson’s ratio. Though the optimum solution provides a quantitatively good agreement, it should always be noted that some other set of microparameters could exist which provide similar or even better agreements. Therefore, the optimality of the solution has to be examined in qualitative way as well and it will be discussed later in this chapter.

As an example to examine the quantitative comparison, results of laboratory test on Wonju granite are set as the target properties to be reproduced (Yoon, 1992). The results from laboratory test are inserted into the optimization problem solver like shown in Figure 2.5 and the optimum microparameters are calculated. The obtained optimum microparameters have to be transformed to uncoded values using transformation equation provided in Table 2.1 and are used as inputs for model generation. Uniaxial compression simulation upon the generated model is carried out and if the discrepancy is within ±5% of relative error range, then we conclude that the model adequately
represent the target rock material. Table 2.8 lists a set of optimum values of microparameters in coded and uncoded format which gives an excellent agreement between the results from laboratory test and those from numerical estimation. The results of the simulations are listed in the last column of Table 2.8. Different packing results in different model strength. Therefore, in order to look into the influence of different packing on the model strength, using the same microparameters, five models with different packing arrangements and microstrengths were created and simulated. The results listed are: mean, standard deviation, variability, and relative error (%). Mean values are 176.3 MPa, 44.7 GPa, and 0.23 for UCS, Young’s modulus, and Poisson’s ratio, respectively. All are within ±5% relative error range and show fair agreements.

Table 2.8 Optimum microparameters for reproducing target physical properties of Wonju granite.

<table>
<thead>
<tr>
<th>Solution</th>
<th>x1 (BCM)</th>
<th>x2 (KNKS)</th>
<th>x3 (FRIC)</th>
<th>x4 (NBS)</th>
<th>x5 (SBS)</th>
<th>x6 (ROSD)</th>
<th>x7 (BRAD)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Coded</td>
<td>0.1017</td>
<td>0.4348</td>
<td>1.0000</td>
<td>0.2713</td>
<td>0.9190</td>
<td>1.0000</td>
<td>0.0298</td>
</tr>
<tr>
<td>Uncoded</td>
<td>73.0510</td>
<td>3.1522</td>
<td>0.7500</td>
<td>145.3475</td>
<td>193.9250</td>
<td>0.4000</td>
<td>0.3636</td>
</tr>
<tr>
<td>[unit]</td>
<td>[GPa]</td>
<td>[---]</td>
<td>[---]</td>
<td>[MPa]</td>
<td>[MPa]</td>
<td>[---]</td>
<td>[mm]</td>
</tr>
</tbody>
</table>

Comparisons between the stress-strain curves from a laboratory test and those from simulation are shown in Figure 2.6. The curves denoted by filled circles represent the data from laboratory test. UCS, Young's modulus and Poisson's ratio are calculated from the stress-strain curve. The elastic constants were obtained for the linear middle portions of the curves. The target UCS, Young's modulus, and Poisson's ratio are 79.0 MPa, 24.9 GPa, and 0.21, respectively. Estimates of UCS, Young's modulus, and Poisson's ratio from simulations on ten different models are shown and they fairly agree. It should be noted that this agreement is achieved by single trial of simulation on the model generated by optimum microparameters. Much more strain is observed at low strain level in the rock specimen due to processes not captured in the bonded particle model, such as grain boundary sliding and closing of pre-existing cracks. Due to the processes, stress-strain curves of laboratory test and simulations look out of accordance. However, this study focused more on matching the peak strength and the intrinsic elastic properties; Young’s modulus, Poisson’s ratio.

The other way of examining the adequacy of microparameters is to compare the mode of failure; e.g. axial splitting, shear localized faulting, brittle and ductile fracturing, and distribution of cracks (diffused or localized), and their propagation patterns, all of which cannot be quantified. Here, in this qualitative verification, an asymmetric triaxial compression test was introduced to demonstrate how the visual comparisons of crack distributions and fracturing patterns are used in proving the
reliability of the developed method. Experimental triaxial rock testing was designed to investigate both pure rock fracture and friction properties (Figure 2.7). The evolution of a fault was technically induced by a triaxial indenter test. The edge of the steel loading plate at the top of the core sample causes a highly stressed region from where a shear rupture is forced to initiate and propagate (Zang et al. 2002).

Figure 2.6 Comparison of stress-strain curves from laboratory test and uniaxial compression simulations on bonded particle models.

Table 2.9 lists the optimum microparameters for generating a model for Aue granite having UCS of 137 MPa, Young's modulus of 70 GPa, and Poisson's ratio of 0.19. Using the microparameters, five models were generated with different particle packing. The imposed constraint comes from the laboratory test that the ratio of $K_{IC}$ to $K_{IIc}$ of Aue granite is 2.6. Table 2.10 lists the results of uniaxial compression simulations, and it shows fair agreement with laboratory test results with relative errors for UCS, Young's modulus, and Poisson's ratio of 5.8%, 7.3%, and 5.0%, respectively.

Table 2.9 Optimum microparameters for Aue granite model and imposed constraint.

<table>
<thead>
<tr>
<th>Microparameter</th>
<th>BCM</th>
<th>KNKS</th>
<th>FRIC</th>
<th>NBS</th>
<th>SBS</th>
<th>ROSD</th>
<th>BRAD</th>
</tr>
</thead>
<tbody>
<tr>
<td>unit</td>
<td>GPa</td>
<td>MPa</td>
<td>MPa</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Value</td>
<td>96.646</td>
<td>2.5167</td>
<td>0.4395</td>
<td>100.0025</td>
<td>200.0000</td>
<td>0.3132</td>
<td>0.2500</td>
</tr>
</tbody>
</table>
| Constraint     | 2SBS/NBS$\leq$3 ($K_{IIc}/K_{IC}$=2.6) [Backers, 2005]
| $K_{IIc}$: Mode II fracture toughness by PTS test method
| $K_{IC}$: Mode I fracture toughness by Chevron Bend method |
Table 2.10 Results of laboratory test on Aue granite and simulations.

<table>
<thead>
<tr>
<th>Property</th>
<th>Aue granite</th>
<th>PFC model (mean ± s.d., coeff. variation, relative error %)</th>
</tr>
</thead>
<tbody>
<tr>
<td>UCS (MPa)</td>
<td>137</td>
<td>144.9 ± 4.5, 0.03, 5.8%</td>
</tr>
<tr>
<td>Young's modulus (GPa)</td>
<td>70</td>
<td>64.9 ± 0.07, 0.01, 7.3%</td>
</tr>
<tr>
<td>Poisson's ratio</td>
<td>0.19</td>
<td>0.20 ± 0.01, 0.05, 5.0%</td>
</tr>
</tbody>
</table>

Traces of rupture paths visible by blue-epoxy impregnation in thin sections of core halves after the tests are shown in Figure 2.8. The sample was tested at 0 and 10 MPa confining pressure. With no confining pressure, the fracture initiated at the high stress concentration point, propagated almost in vertical direction and slowly curved out to the unloaded portion of the sample (Figure 2.8a). At 10 MPa confining pressure, the fracture also started at the tip of the steel loading plate, but as it propagated, it turned its direction to the loaded portion of the sample (Figure 2.8c). The surface of the rupture with no confinement exhibited clean faces with mostly inter-granular cracks. In the sample under 10 MPa confining pressure, however, along the rupture path, a wide process zone was formed having many sub-vertical and en échelon cracks. This indicates that severe confined frictional sliding followed the fracturing of the sample.

Those rupture traces were reproduced in the simulations on the PFC model generated using the microparameters listed in Table 2.9. With no confinement, the cracks are clustered at the place of high stress concentration. The width of the crack cluster later becomes narrower at it curves out to the unloaded portion of the mode, and it can be seen by the black segments that most of the cracks are tensile types (Figure 2.8b). At 10 MPa confining pressure, a wider crack cluster is formed, which is supported by the experimental observation. Along the path, not only tensile cracks but also shear cracks (red segments) were formed, which indicates that the two blocks were sheared against each other (Figure 2.8d). Comparison of the pictures reveals that the microparameters listed in Table 2.9 are adequate to be used in model generation for Aue granite. It should be understood that this agreement of crack distributions was made possible because the model was appropriately generated by the microparameters obtained using the imposed constraint, which is deduced from considering the ratio of $K_{Ic}$ to $K_{IIc}$ of Aue granite.

2.7 Conclusions

A new method of microparameter determination for bonded particle model generation was introduced, which incorporates methods of Design of Experiment and optimization. One of the distinctive advantages of the new method is that by inserting proper constraints, we can regulate the solution, so that the intrinsic properties of rock material could be reflected in the process of microparameter determination and a tailor-made contact bond particle model could be generated. It turned out that the microparameters provided not only quantitative matching of the UCS, Young's
modulus, and Poisson’s ratio but also qualitative matching, as revealed by comparisons of crack distribution. This proves conclusively the reliability of the developed method for the determination of microparameters for model generation.

**Figure 2.7** Photograph of Aue granite sample with principal loading configuration in asymmetric compression test and its two dimensional schematic representation (cross-sectional view A-A’).

**Figure 2.8** Rupture paths in thin sections visible by blue-epoxy impregnation and crack distributions in model of Aue granite at zero (a,b) and 10 MPa confining pressure (c,d).
Many geophysical processes and a large number of geotechnical problems embody coupling between solid and fluid, either in forms of pore fluid or flow through discontinuities. Therefore, understanding of mechanical properties of rocks under the presence of pore fluid pressure is important in rock engineering 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 confining pressure. 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 rock is subjected to stress, multiple cracks nucleate, propagate, interact and coalesce, which induces change of the pore fluid pressure in the rock. This complex multiplicity of fracture interacting events also causes the 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 to simulate solid-fluid coupling using various numerical schemes. Among those, Sakaguchi and Mühlhaus (2000) developed a hybrid formulation for coupled solid particle pore fluid deformation and the potential of their new method was illustrated by example solutions related to failure and localization in brittle materials under undrained biaxial compression which turned out to be successful. The present work uses similar formulation for pore fluid generation and for calculation of solid-fluid interaction. In this technique, fluid is assigned to actual voids formed by surrounding adjacent solid particles, and flows between neighboring voids according to the hydraulic gradient. The apparent area of a pipe, which is formed between neighboring voids, is variable according to contact conditions between the particles forming the pipe. Figure 3.1 presents fluid contained in voids between solid particles. Fluids are denoted by yellow dots and are contained in black polygons. Fluid flow between two neighboring voids only occurs through a pipe denoted by red color.

This chapter deals with simulation of hydro-mechanical coupling in bonded particle model. Development of the hydro-mechanical coupling is based on the formerly proposed algorithm by Cundall (2000) and laster modified by Hazzard et el. (2002) using the conventional particle based modeling. It is applied to simulation of biaxial compression tests. Variation of strength and seismic characteristics under pore fluid pressure are investigated and compared with theoretical and
3.1 Coupling of solid particles and pore fluids

3.1.1 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. 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 3.1).

3.1.2 Formulation of fluid flow

Fluid formulation regards the void geometry in an assembly of circular particles as being identical to the actual space between particles. Here, it is assumed that the assembly represents a material of low porosity, such as granite. Each link termed a pipe between two adjacent domains is a potential crack, because it corresponds to a bonded contact that may break. Based on the former fluid flow algorithms proposed by Cundall (2000) and Hazzard et al. (2002) some modifications have been made. The fluid algorithm assumes that the bonded particle model is made up of a series of channels or pipes 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

Figure 3.1 Representation of solid particles and network of pore fluids (yellow dots) contained in voids between solid particles. Fluid flows through the pipes denoted by red segments.
is, therefore

\[ Q = \frac{a^3 \Delta P}{12 \mu L} \]  \hspace{1cm} (3.1)

where, ‘a’ is the aperture, ‘\( \Delta P \)’ is the pressure difference between domains, ‘\( \mu \)’ is dynamic viscosity of the fluid and ‘L’ is the length of the 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

\[ a = \frac{a_0 F_0}{F + F_0} \]  \hspace{1cm} (3.2)

where, ‘\( a_0 \)’ is the residual aperture and ‘\( F_0 \)’ is the 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 time steps. Each domain receives flow from the surrounding pipes. In one time step, \( \Delta t \), the change in fluid pressure is given by:

\[ \Delta P = \frac{K}{V_d} \left( \sum Q \Delta t - \Delta V_d \right) \]  \hspace{1cm} (3.3)

where, ‘\( K \)’ is the fluid bulk modulus and ‘\( V_d \)’ is the volume of 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 open pipes in which particles are not touching, equation (3.3) is bypassed and the pressure in each of the joined domains is set to the average pressure of the two domains (Hazzard et al., 2002). This essentially assumes that the pipe has an infinite permeability. This fluid flow algorithm is a modified form of the technique proposed by Cundall (2000). The main modification done by Hazzard et al. (2002) 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 is reduced to zero.

### 3.1.3 Aperture calculation
Darcy’s law for a linear porous medium is expressed as:

\[ q_i = \frac{k_i}{\mu} \frac{\partial P}{\partial x_i} \quad (3.4) \]

where, ‘\( q_i \)’ is the one-dimensional flow rate (units of velocity), ‘\( k_i \)’ is the permeability and ‘\( \mu \)’ 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, ‘\( V \)’:

\[ \bar{q} = \frac{1}{V} \sum_{\text{pipes}} q^p V^p \quad (3.5) \]

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 (3.1) by the pipe cross-sectional area ‘\( A^p \)’,

\[ q^p = \frac{a^i \Delta P n_i}{12 \mu L A^p} \quad (3.6) \]

where, \( n_i \) is an unit vector. Substitute into equation (3.5),

\[ \bar{q} = \frac{1}{V} \sum_{\text{pipes}} \frac{1}{12 \mu} a^i \Delta P n_i \quad (3.7) \]

The pressure difference between two points separated by vector distance ‘\( L n_i \)’ is:

\[ \Delta P = L n_i \frac{\partial P}{\partial x_i} \quad (3.8) \]

Substituting in equation (3.7),

\[ \bar{q} = \frac{1}{V} \frac{\partial P}{\partial x_i} \sum_{\text{pipes}} \frac{1}{12 \mu} a^i L n_i \quad (3.9) \]

Comparing with equation (3.1), the permeability can be expressed as,

\[ k_i = \frac{1}{V} \sum_{\text{pipes}} \frac{1}{12} a^i L n_i \quad (3.10) \]

In the special case of an isotropic medium where, \( n_i = n_1 \), leading to \( n_i n_i = 1 \)

\[ \bar{k} = \frac{1}{2} k_0 = \frac{1}{24 V} \sum_{\text{pipes}} a^i L \quad (3.11) \]
We can calculate the total volume of the assembly by taking the sum of particle volumes and dividing by $1-n$, where ‘$n$’ is the mean porosity. Equation (3.11), then becomes,

$$k = \frac{1-n}{24\pi} \sum_{\text{pipes}} \frac{R^2}{La^3} \quad (3.12)$$

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:

$$a = \sqrt[3]{\frac{24\pi}{(1-n) \sum_{\text{pipes}}} \sum_{\text{balls}} R^2} \quad (3.13)$$

In this way, the residual aperture required for a given permeability can be estimated. Figure 3.2 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 (3.1) 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. It is referred to residual aperture and it is expressed by equation (3.13). As shown in Figure 3.2, 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 (3.2). However, when there is tensile force at the contact, i.e. when they are separated, 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. This is undesirable for the stability of numerical calculation. When the tensile contact force is further increased, then the contact experiences bond breakage. Even in this case, the residual aperture is still used for volumetric fluid flow calculation.

Exertion of traction forces by domain pressure on the enclosing particles is described in Figure 3.3. It is assumed that the pressure drop due to flow through a pipe is localized at the corresponding contact. The pressure in the region of the domain is uniform, and the tractions are independent of the path around the domain. The polygonal path that joins the contacts defines a domain. The force vector on a typical particle is:

$$F = Pn_s \quad (3.14)$$

where, $n_s$ is the unit normal vector of the line joining the two contact points on the particles, and $s$ is the length of the line. Interaction of pore fluid and particles takes place in sequence as listed in Figure 3.3. External force causes particle displacement, then it triggers domain pressure
disturbance and generates pressure gradient between nearby pores. Fluid then starts to flow, and it causes domain volume disturbance, and subsequently, domain pressure is disturbed, and it goes back to particle displacements. It keeps cycling until the model reaches equilibrium state.

![Diagram](image1.png)

**Figure 3.2** Variation of aperture value at contact. Residual aperture is defined as the aperture when the two particles are touching without any compression or tension.

3.2 Verification problems

3.2.1 Pore fluid permeation

The coupling scheme uses Darcy's law for the fluid flow between domains through the pipes connecting the adjacent domains. A rectangular model (50 mm width and 100 mm height) is generated in which particle movements are restricted by four confining walls. To consider the case of water saturation, the pore fluid in the model is initially pressurized with 0.1 MPa, i.e. 0.1 MPa is
assigned to each domain pressure, identical to atmospheric pressure. At the top boundary, 5 MPa pore fluid pressure is applied and maintained throughout the cycling. Initially the high pressure gradient is concentrated in the vicinity of the upper boundary, and the body forces induced by the local pore fluid pressures result in the local consolidation of fluid in vertical direction. Two different rock models were considered. A granite model and a sandstone model have different residual aperture values which are calculated by permeability calculation following the procedure presented previously assuming that the desired macro permeability (unit of Darcy flux) of granite and sandstone are $5 \times 10^{-19}$ m/sec and $5 \times 10^{-15}$ m/sec. The residual apertures of granite and sandstone models are 0.253 and 5.447 microns, respectively. Due to the difference of these residual apertures, different speeds of water permeation were simulated in granite and sandstone models. This can be checked by observing the water permeation front moving in vertical direction. Figure 3.4 shows front of pore fluid permeation moving in two different models but at the same calculation time steps. On these two models, constant fluid pressure was applied on the upper part of these two models, and as time goes fluid permeates through apertures and moves down. But in the sandstone model, this process is much faster.

3.2.2 Biaxial compression simulation

The coupling scheme is applied to a series of biaxial compression simulation. The top and bottom boundaries simulate loading platens in a strain-controlled condition. Results of biaxial compression simulations are compared to those from the uncoupled (mechanical only) simulation on Aue granite models. Also, the numerical moment tensor inversion technique is implemented in order to look into the seismic characteristics of crack events focusing on b-value variations in rock model where internal pore fluid pressure is acting.

In the following series of bonded particle model simulation, samples of Aue granite are simulated of which the microparameters are mentioned in the previous chapter. Pore fluid in a domain tends to push the surrounding particles away. When the two adjacent particles are pushed away, the gap (aperture) between these two particles increases which eventually causes fluid flow to occur. Increased pore fluid pressure results in weaker contact force chain. Fluid flows through the increased aperture and this causes reduction of inter-particle friction between the two touching particles by lubrication due to the fluid (Baud et al., 2000). Distribution of inter-particle friction coefficients in the models when the pore fluids (domains) are pressurized with 1, 3, 5, 10 MPa are shown in Figure 3.5. It is clearly shown that the pore fluid pressure results in fluid flow in the vicinity of the sample boundaries and reduces inter-particle friction coefficients.
Figure 3.4 Permeation of pore fluids in granite and sandstone models.
Figure 3.5 Distributions of inter-particle friction coefficient in granite model at different levels of pore fluid pressures.

Strength envelopes presented by Mohr circles are shown in Figure 3.6. The Mohr-Coulomb envelopes are achieved from biaxial compression tests under pore fluid pressures of 1, 3, 5, 10 MPa together with the results from uncoupled simulation presented previously. Assuming that the models are equivalent to Mohr-Coulomb materials, macroproperties of the models under different pore fluid pressure are obtained (Table 3.1). These results indicate that the angle of internal friction and cohesion are strongly influenced by presence of pore fluid pressure. However, little difference is observed between the models for 1, 3, 5, 10 MPa pore fluid pressure.

Table 3.1 Friction angle and cohesion of granite model from biaxial compression simulations.

<table>
<thead>
<tr>
<th>Pore fluid pressure (MPa)</th>
<th>Friction angle (degree)</th>
<th>Cohesion (MPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>22.6</td>
<td>40.2</td>
</tr>
<tr>
<td>1</td>
<td>15.8</td>
<td>41.8</td>
</tr>
<tr>
<td>3</td>
<td>13.9</td>
<td>43.7</td>
</tr>
<tr>
<td>5</td>
<td>16.3</td>
<td>40.3</td>
</tr>
<tr>
<td>10</td>
<td>14.0</td>
<td>42.1</td>
</tr>
</tbody>
</table>

Figure 3.6 Mohr circles for granite model in biaxial compression simulations subjected to pore fluid pressures.
Figure 3.7 shows crack distributions and pore fluid concentrations after the models have reached 80% of their peak strength confined with 15 MPa confining pressure but subjected to different pore fluid pressure, which resulted in different effective confining pressure; (a) 14 MPa, (b) 12 MPa, (c) 10 MPa, (d) 5 MPa. Due to different magnitude of effective confining pressure, different strengths were obtained; (a) 138.44 MPa, (b) 137.48 MPa, (c) 135.06 MPa, (d) 130.77 MPa. Also, one can notice herein that at high effective confining pressure, cracks are localized in a major fracture, and at low confining pressure cracks are distributed in a more diffused way. Moreover, in Figure 3.7d a few vertically oriented fractures are observed. From the figures showing pore fluid concentration, it is observed that pore fluids are concentrated along the major fracture (Figure 3.7a). This happens because there is a strong pressure gradient between parts being compacted and parts being dilated. Local pore fluid exchanges occur between these two parts. These numerical simulation results are consistent with the laboratory experimental findings by Sulem and Ouffroukh (2006), who have done a detailed analysis of shear band formed in drained and undrained triaxial test on Fontainebleau sandstone. They have shown that local fluid exchanges occur where the shear band is formed.

Figure 3.7 Crack distributions and pore fluid concentration in granite models confined by 15 MPa confining pressure and subjected to four levels of pore fluid pressure.
Seismic magnitudes of crack sources are monitored. The cumulative number of crack events is plotted against magnitude in Figure 3.8 for the cases when the confining pressure is 40 MPa with 1, 3, 5, 10 MPa pore fluid pressure together with uncoupled case. Slopes of the linear part of the curves are defined as b-values. In seismology, b-value is derived from the amplitude distribution data of acoustic emission. The b-value is defined as the log-linear slope of the frequency-magnitude distribution which is found to obey the Gutenberg-Richter relation (Gutenberg & Richter, 1954), i.e. \( \log N = a + bM \), where \( N \) is the number of events which occurred of magnitude \( M \), and \( a \) and \( b \) constants (Figure 3.8). A high b-value arises due to a large number of small AE 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 AE in larger numbers (Rao & Prasanna Lakshmi, 2005). When the pore fluids are pressurized, they will act as wedges. This 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 AE which will eventually leads to low b-values. In Figure 3.8, the magnitude limits are restricted to the range between -4.50 and -4.75, where there are enough statistical data points. As the figure shows, b-value decreases as the pore fluid pressure increases for one and the same confining pressure. This supports the hypothesis presented earlier that pore fluid pressure enhances faster and unstable crack growth. Differences of b-values for dry and wet sample conditions are experimentally verified by Zang et al. (1996). They performed uniaxial compression tests on dry and wet Flechtingen sandstones and calculated b-values from AE pulse statistics and 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 hypothesis presented above and eventually leads to conclusion that the developed hydro-mechanical coupling scheme provides reasonable basis for modeling strength and seismic characteristics of saturated rock.

3.3 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 described. 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 migration plays a crucial role on the fracture propagation in water saturated rocks.
The following conclusions are drawn.

1) Modeling of coupled interaction between pore fluids and solid particles is formulated. This hydro-mechanical coupling 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. The effect of pore fluid on strength has been well reproduced both in biaxial compression simulations.

2) Seismic characteristics of crack events are monitored and analyzed. Calculated b-values in dry, and pore fluid pressurized rock models exhibited similar tendency as is observed in seismology. Introduction of pore fluids accelerates the failure process of 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.

Figure 3.8 Frequency-magnitude plots of seismic sources for granite models subjected to 40 MPa confining pressures under four levels (0, 1, 3, 5, 10 MPa) of pore fluid pressure.
4. NUMERICAL AND EXPERIMENTAL STUDIES ON CONFINED SHEAR-INDUCED FRACTURING OF ROCKS

This chapter presents Punch Through Shear test. It starts with the bonded particle modeling of PTS test using the hydro-mechanical coupling presented in chapter 3. Simulation results are used as estimations for laboratory tests and they are later compared.

4.1 Bonded particle modeling of PTS test

Figure 4.1 presents the sample geometry and principle loading for PTS test. Each step of numerical procedure in simulation is described with corresponding figures in Figure 4.2. A model is generated so that it has the strength and permeability characteristics of granite. Next, particles comprising region 1, 2, 3, 4 are deleted to make traction free initial notches with thickness of 1.5 mm (Figure 4.2a). Particles in region 5 are also deleted to give enough space for the displacement of the inner cylinder being punched down. Domains are initially pressurized with 0.1 MPa pressure in order to simulate model saturation (Figure 4.2c). Axial centered loading on wall 2 is applied downward with 0.05 m/sec speed. Figure 4.2d shows the crack distributions in the model at failure.

![Sample Geometry and Principle Loading](image)

(a) Sample geometry in 3D  (b) Cross-sectional view

**Figure 4.1** Suggested sample geometry in 3D view (a) and cross-sectional view (A-A') with principle loading configuration (b). Inner diameter (ID): 25 mm; Outer diameter (W): 50 mm; Sample height (H): 50 mm; Top notch depth (a): 5 mm; Bottom notch depth (b): 30 mm; Notch thickness (t): 1.5 mm.
In the simulations, two model conditions are concerned; dry and saturated. Dry condition is merely represented by uncoupled, i.e. mechanical only, simulation. Mechanical data from the simulation of two different model conditions are compared. They include axial force variation, and evolution of cracks and process zone.

4.2 Simulation results – Effect of presence of pore fluid

Two axial load versus axial displacement curves of PTS simulations are shown in Figure 4.3 in
which one represents dry model case and the other represents saturated model case both subjected to 5 MPa confining pressure. A prominent difference in peak load is noticed. In the dry model, the peak axial load is about 150 kN, whereas in the saturated model it is 130 kN. This is attributed to strength weakening due to presence of pore fluid. This mechanical effect is attributed to increase in pore fluid pressure which reduces the effective confining pressure, and decrease of inter-particle friction coefficients which reduces the frictional resistance between particles.

![Figure 4.3 Axial force versus axial displacement curve of PTS simulation for dry and saturated models both subjected to 5 MPa confining pressure.](image)

Two curves are subdivided into 3 stages (stage 1: linear pre-peak; stage 2: nonlinear post-peak; stage 3: nonlinear failure post-peak and residual). In stage 1, the axial load increases more or less linearly and shows very small load drops. At stage 1, small number of cracks initiated at the tip of the bottom notches (Figure 4.4a, d). Stage 2 is characterized by formation of major fracture connecting the two sample notches which leads to sudden drop of axial force (Figure 4.4b, e). In dry model, force drops but it recovers slowly and major fracture connecting upper and bottom notches are formed. However in case of saturated model, the force drop is rapid. This difference is attributed to the presence of pore fluid, which migrates to open cracks and reduces the inter-particle friction. This effect could be interpreted in a physical sense that when microcracks are generated and interconnected into a cluster of cracks in the saturated medium, pore fluids are concentrated at the crack cluster by suction of pore fluids into this crack cluster from neighboring pores. Pore fluid migration happens due to pressure gradient between the two zones formed in the model; one being
compacted and expels fluids and the other being dilated and absorbs fluids (Figure 4.8). Pore fluids migrate into the growing fracture and lubricate the fracture surface and eventually reduce the frictional resistance between grains and crack surfaces. In the dry model, the axial load is mostly lost during stage 3 which exhibits sudden load drop. However, this load drop is attributed to failure of outer ring of the model and it is not related to the failure of the intact part between the two sample notches which is the intended failure of PTS test.

Peak axial load both in dry and saturated models subjected to various confining pressures are recorded as 10~20%. Introduction of pore fluid results in peak axial load decrease. In rock mechanics, the influence of the moisture content (presence of pore fluid) is well known regarding its effect on the strength and deformation characteristics of rocks (Alm, 1982; Rao et al., 1987; Choi et al., 1988). Hoagland et al. (1973) showed that with the introduction of water, surface energy was over 30% lower than that obtained under ambient conditions. Experimental data supporting this are provided by Backers (2006). He has performed a series of $K_{IC}$ and $K_{IIC}$ tests using Chevron-Bend method and Punch Through Shear method, respectively on both dry and saturated Åspö diorite. His data are compiled in Table 4.1. Data show that in saturated condition, $K_{IC}$ and $K_{IIC}$ exhibit 14.4~27.9% and 12.5% of reduction, respectively.

| Table 4.1 Mode I and II fracture toughness data of Åspö diorite. |
|-----------------|-----------------|-----------------|
| **Testing**     | **Parameter**   | **Value**       | **Reference**   |
| Chevron Bend method | $K_{IC}$ - dry  | 3.80 MPa\(\sqrt{m}\) | Backers, 2005   |
|                  | $K_{IC}$ - dry  | 3.20 MPa\(\sqrt{m}\) | Staub et al., 2003 |
|                  | $K_{IC}$ - saturated | 2.74 MPa\(\sqrt{m}\) | Backers, 2006   |
| Punch Through Shear method | $K_{IIC}$ - dry | 5.10 MPa\(\sqrt{m}\) | Backers, 2005   |
|                  | $K_{IIC}$ - saturated | 4.46 MPa\(\sqrt{m}\) | Backers, 2006   |

Fracture patterns at two confining pressure are shown in Figure 4.5. Backers et al. (2000) drew a conclusion that tensile crack propagation is increasingly suppressed with confining pressure increase. The increase of confining pressure enhances the ‘pureness’ of mode II in the fracturing process. In PTS testing, a wing fracture develops at the bottom notch first, but elevated confining pressure suppresses these wing fractures. At low confining pressure, wing fractures which initiate at the inner tip of the bottom notch and progress into inner cylinder part are observed. For high confining pressure regime, these wing fractures are not observed (Figure 4.5a, b). In saturated models, however, those wing fractures are less observed either in case of low or high confining pressure. This difference is attributed to presence of pore fluid pressure.
Difference in the size of damage zone (width of crack cluster) is noticed from Figure 4.5b, d. The width of crack cluster in the saturated model is bigger than that in dry model. This is explained by the concept of Fracture Process Zone (FPZ). In rock materials, the process zone is caused by
initiation and propagation of the microcracks in the immediate vicinity of a crack tip. Consequently, it is described as FPZ. Characteristics of the FPZ including zone size and how it is formed might be affected by the presence of pore fluid. In PTS simulation, before the onset of unstable crack initiation and propagation which finally grows into macrofracture connecting the top and bottom notches, a FPZ is gradually formed at the vicinity of the bottom notch tip by the existing and newly produced microcracks initiating, propagating and interacting and/or linking.

Introduction of pore fluid can have significant and/or insignificant influence on FPZ formation. As the specimen is loaded, an isolated microcrack is connected to another adjacent isolated microcrack. This process continues until microcracks are clustered and grow into a size of FPZ. When the FPZ is formed, pore fluids adjacent to this FPZ are sucked into it. This could be understood intuitively because of pressure gradient between the compacting zone and dilating zone (Figure 4.8). Suction of pore fluids into the FPZ reduces the effective confining pressure acting upon the FPZ. Equation expressing the characteristic FPZ size is formulated by Schmidt (1980) based on the maximum normal stress criterion applied to mode II crack propagation and it is expressed by the following equation.

\[ r_0 = \frac{1}{2\pi} \left( \frac{K_{II}}{\sigma_u + \sigma_u - p_u} \right)^2 \left[ -\sin \theta + \frac{1}{2} \sqrt{1 + 3 \cos^2 \theta} \right]^2 \]  \hspace{1cm} (4.1)

where, ‘\( r_0 \)’ is the radius of characteristic FPZ size, ‘\( \sigma_u \)’ is uniaxial tensile strength, and ‘\( \sigma_u - p_u \)’ is effective confining pressure (confining pressure - pore fluid pressure), and \( K_{II} \) is mode II stress intensity factor. When pore fluids are sucked into the FPZ, then this will reduce the effective confining pressure, which according to equation (4.1) reduces the denominator and eventually leads to increase of the radius of characteristic FPZ size. Therefore, it can be said that introduction of pore fluids leads to wider fracture process zone.
4.3 Laboratory PTS test

Mode II fracture propagation was technically induced by PTS test (Backers, 2005). The PTS test uses cylindrical samples with circular notches drilled centered into the end surfaces where the notches serve as friction free initiation locus for fracture. The suggested sample geometry, its dimension and principle loading are given in Figure 4.1. Tested material is Daejeon granite and their mechanical properties are listed in Table 4.2.

Table 4.2 Physical properties of Daejeon granite.

<table>
<thead>
<tr>
<th>Properties</th>
<th>Daejeon granite</th>
</tr>
</thead>
<tbody>
<tr>
<td>Uniaxial compressive strength</td>
<td>150 MPa</td>
</tr>
<tr>
<td>Young's modulus</td>
<td>59 GPa</td>
</tr>
<tr>
<td>Poisson's ratio</td>
<td>0.22</td>
</tr>
<tr>
<td>Tensile strength</td>
<td>8.7 MPa</td>
</tr>
<tr>
<td>Specific gravity</td>
<td>2.64</td>
</tr>
<tr>
<td>Porosity</td>
<td>0.7 %</td>
</tr>
</tbody>
</table>
From a drill core, samples of length 50 mm are cut. The end surfaces are ground to provide flat end surfaces perpendicular to the core mantle. In PTS test sample preparation, it is crucial to drill top notch and bottom notch so that both are concentric circles. The circular notches of width 1.5 mm are drilled. The prepared sample is placed between bottom support and loading stamp assembly. The assembly with sample is placed into a Hoek cell. Special devices were developed which are designed to work with a conventional Hoek cell. The bottom support is a solid cylinder and it supports the outer bottom ring of the sample during testing, while the central bottom part is unconstrained. Schematics of the devices can be referred to the provided references (Backers, 2001; Backers et al., 2002; Stephansson et al., 2001; Yoon, 2002b; Yoon & Jeon, 2003; 2004).

Prior to the actual testing procedure, a small pre-load is added to the stamp to provide good adjustment. Confining pressure is applied and then the inner cylinder of the sample is then punched down at a constant displacement rate control. The applied axial stress generates an increasing shear stress in the intact rock portion between the notches until failure. Axial force and axial displacement are recorded. Two sample conditions are considered, i.e. dry and wet. Five levels of confining pressure applied in PTS test: 0, 2.5, 5, 7.5, 10 MPa. Three different loading speeds are applied: 0.2, 0.1, 0.02 mm/min. Axial peak load variations of granite samples under the presence of pore fluid are analyzed.

4.4 Experimental results – Effect of saturation

Peak axial force and $K_{IC}$ variation in saturated conditions are listed in Table 4.3. Reduction of peak axial force and fracture toughness are also listed. Backers (2005) suggested the generalized formulation for determination of the fracture toughness given in the form

$$K_{IC} = 0.0378 \cdot \sigma_{\text{atm}} \cdot 1.795 \cdot 10^{-3} \cdot P_{\text{con}}$$

where, ‘$\sigma_{\text{atm}}$’ is the axial load at failure, ‘$P_{\text{con}}$’ is the applied confining pressure.

Table 4.3 Peak axial force and $K_{IC}$ data in PTS tests for granite at five levels of confining pressures.

<table>
<thead>
<tr>
<th>Confining pressure</th>
<th>Dry Peak load (kN)</th>
<th>Saturated Peak load (kN)</th>
<th>Reduction</th>
</tr>
</thead>
<tbody>
<tr>
<td>0 MPa</td>
<td>43.8</td>
<td>33.3</td>
<td>24%</td>
</tr>
<tr>
<td>2.5 MPa</td>
<td>62.9</td>
<td>55.2</td>
<td>13%</td>
</tr>
<tr>
<td>5 MPa</td>
<td>78.7</td>
<td>71.5</td>
<td>10%</td>
</tr>
<tr>
<td>7.5 MPa</td>
<td>87.5</td>
<td>80.9</td>
<td>8%</td>
</tr>
<tr>
<td>10 MPa</td>
<td>139.8</td>
<td>107.5</td>
<td>23%</td>
</tr>
</tbody>
</table>

4.4.1 Effect of saturation on strength and deformation

Axial force versus axial displacement curves for granite samples in dry and saturated conditions
under three levels of confining pressures: 0, 5, 10 MPa, are given in Figure 4.6. In saturated condition, the slope of the linear part of the curves is reduced compared to the curves in dry condition. This stiffness difference is attributed to presence of pore fluid. This stiffness reduction has been estimated by simulation shown in Figure 4.3. $K_{IC}$ variations under confining pressure up to 10 MPa in dry and saturated granite samples are recorded at about 10~20% loss (Table 4.3). The amount of reduction was estimated previously in the simulation, which was 10~20%. The bonded particle models simulated were treated as granite samples. Comparison between the results from experiments and simulations shows good agreements.

Figure 4.7 shows two different axial load versus displacement curves for dry and saturated granite at 7.5 MPa confining pressure. Saturation reduces the slope of load-displacement curve in the pre-peak loading regime. After the samples have failed they exhibited rapid load drops which are caused by formation of major fractures connecting the two sample notches. However, from the point where brittle load drop stops, different unloading stiffness in dry condition and saturated condition is measured. The unloading stiffness in dry condition, stiffA, is little bit bigger than that in saturated condition. Backers (2005) has performed repeated loading on various rock types in dry sample condition. He calculated the slopes of loading/unloading/reloading loops and presented them respect to axial force. He separated the change in rock stiffness during loading/unloading cycles into four distinct regimes as follows.

Regime 1: Up to 80% of the maximum load, stiffness consistent with linear elastic part of the curve, no significant cracking.

Regime 2: Stiffness decreases considerably above the yield point, process zone formation. Fracture propagates, stiffness decreases as the intact portion becomes shorter.

Regime 3: In between Regime 2 and 4, two mechanisms of fracture propagation and interlocking superimpose, apparent constant stiffness.

Regime 4: Stiffness increase below 60% of peak stress in the post peak region due to interlocking of the mode II fracture faces, grain rotation and compaction. The interlocked grains of the rough fracture faces are pressed against each other by shear displacement.

In Figure 4.7, the stiffness increase in the post-peak loading regime is observed. Both two samples exhibit stiffness increase. However, the sample under saturated condition exhibits lower stiffness than the one in the dry sample. Interlocking of the fractured surfaces, grain rotation, compaction, which are the characteristics of the stiffness increase in the regime 4 might have been affected by
the presence of pore fluid. Fracture interlocking, grain and rock fragment rotation in the fractured faces results in stiffness increase as the inner cylinder part is displaced by shearing. This could be even more pronounced at higher confining pressure. Before the major fractures are formed, there exist local pore fluid exchanges between the compacting zone and the crack opening zone being dilated which absorbs fluid. As the macro-fracture develops and advances ahead of process zone, pore fluids permeate and are concentrated in the region where fracture faces are formed. Fluid concentration in the fractured region lubricates the fracture surfaces (inter-granular and/or intra-granular boundaries) and hence provides mobility of the interlocking of the fractured surfaces. Grain rotation also could be affected by the fluid. This mechanism could be the possible explanation for the stiffness difference in the post-peak loading regime.

4.4.2 Effect of loading rate on strength in saturated condition

The displacement rate controlled loading was varied between 0.02, 0.2 mm/min for dry and saturated granite and sandstone at 5 MPa confining pressure. The axial peak load variation in granite samples under different loading rates are presented in Figure 4.8. In case of granite, peak axial load decreased from 71.5 kN at dry sample condition to 64.3 kN at saturated condition. A prominent difference in axial load versus axial displacement curves are noticed between granite cases under different loading rates. In Figure 4.8a for the case of granite, there is not much difference in stiffness of the linear parts of the two curves, one for 0.2 mm/min loading rate and the other for 0.02 mm/min loading rate. But for the case of sandstone, stiffness is much reduced. This difference is attributed to porosity difference between granite and sandstone. When a saturated sample undergoes punch loading, two zones are formed within the sample, one being compacted and the other being dilated. Pore fluid migration and local exchange occur between these two zones through the rock matrix which is located between the two zones. In case of granite, pore fluid permeation takes much more time to travel from the compacting zone through the rock matrix to reach the dilating zone due to low porosity. In sandstone, pore fluid migration through a more porous rock matrix takes less time compared to that in granite, hence it can easily degrade the strength of the rock matrix and results in less initial stiffness (Figure 4.8b).
4.4.3 Fracture inspection

Fracture traces were inspected. The failed samples were soaked in and coated with epoxy resin and cut parallel to the fracture plane. Shear fracture consists of, irrespective of the magnitude of confining pressure, a narrow zone of branching, predominantly intra- and trans-granular microcracks (Backers, 2005), referred to in the following as main fracture, and an array of inclined (en échelon) and sub-parallel fractures (Figure 4.9). Figure 4.10 shows the pattern of fracture coalescence in granite samples under dry and saturated conditions, subjected to 5 MPa confining pressure. In dry condition, a distinct wing fracture is observed which initiated at the bottom inner notch tip. Main shear fracture was generated connecting the bottom outer notch tip and the top inner notch tip, which is formed by coalescence of en échelon fractures. Sub-parallel fractures are also shown (Figure 4.10a).

What happens when the sample is saturated is of concern. Figure 4.10b shows the fracture traces making up the main shear fracture initiated at the bottom outer notch tip. In saturated condition, sub-parallel fractures are aligned in a wider zone. According to Backers’ statement (Backers, 2005), the shear fracture process zone is defined as a zone in which intact rock portion is severely damaged by formation of cracks/fractures and their coalescences into main shear fracture. The cracks and fractures making up the process zone include sub-parallel cracks, en échelon cracks and main shear fracture (Figure 4.9). Therefore, according to the definition of width of process zone, bigger width of the process zone is resulted from the saturation effect. This is consistent to the theoretical explanation based on the equation formulated by Schmidt (1980) explaining the

Figure 4.6 Axial force versus axial displacement curves for granite in dry and saturated conditions.
characteristic size of FPZ under the circumstance of mode II crack propagation, equation (4.1). According to his formulation, when pore fluids are sucked into the FPZ, then this will reduce the effective confining pressure, which according to equation (4.1) reduces the denominator and eventually leads to increase of the radius of characteristic FPZ size. Therefore, introduction of pore fluids leads to wider fracture process zone.

Figure 4.7 Slope of unloading portion (post-peak region) in dry and saturated sample conditions subjected to 7.5 MPa confining pressure (a), fractures formed in zigzag patterns with grains and rock fragments coming off from the fracture surfaces (b).
(a) axial load versus axial displacement curves for Daejeon granite and Bentheimer sandstone at two loading rates

(b) formation of compacting zone and dilating zone and pore fluid migration through rock matrix

Figure 4.8 Axial force versus axial displacement data for Daejeon granite and Bentheimer sandstone in dry and saturated conditions under two different loading rates (0.2, 0.02 mm/min) (a) and pore fluid migration from compacting zone through rock matrix to dilating zone (b).
Figure 4.9 Schematic drawing of the main shear fracture and process zone at the bottom notch with inclined (en échelon) and sub-parallel cracks (Backers, 2005).

Figure 4.10 Fracture traces in failed granite samples in dry and saturated conditions subjected to 5 MPa confining pressure.
4.5 Conclusions

In this chapter, mode II fracturing processes in dry and saturated rocks were tested. Mode II fracture was technically induced by Punch Through Shear test proposed by Backers (2005). The objective of this chapter is to carry out PTS experiments on dry and saturated rocks and to compare the results to those obtained by hydro-mechanical coupled bonded particle model simulations. It turned out that some of the results are quantitatively consistent with the estimations.

The following conclusions were drawn in this chapter.

1) The developed hydro-mechanical coupling is applied to simulation of PTS test. It is observed that the peak strength was reduced 20% due to the presence of pore fluid. The fluid concentration into the local cracks takes part in further propagation and branching of the crack and development of process zone.

2) In laboratory PTS experiments, the reduction of peak axial force and mode II fracture toughness in granite were recorded as 10~20%. These results were consistent with the estimation made by PTS simulations.

3) Peak axial load variation in granite and sandstone under different loading rates were examined. A prominent difference in axial load versus axial displacement curves were noticed between granite and sandstone cases under different loading rates. This difference is attributed to porosity difference, and pore fluid migration through the rock matrix which is located between the compacting zone and the dilating zone. In case of granite, pore fluid permeation takes much more time to travel from the compacting zone through the rock matrix to reach the dilating zone due to low porosity, hence smaller chance for degrading the rock matrix’s strength.

4) Fracture traces were inspected. Fractures in saturated granite samples exhibited a wider zone compared with the dry sample.
5. SUMMARY

A new method for determining microparameters for generation of a contact bond model was developed in which Design of Experiment and optimization were used. By Plackett-Burman design, the sensitivity of microparameters to macroscopic responses was quantified and for each macroscopic response, two microparameters having the biggest impacts were selected. Central Composite Design method was then used to estimate the non-linear relations between the two selected microparameters and the macroscopic responses. Quantified linear and non-linear relations between microparameters and macroscopic responses resulted from Plackett-Burman design and from Central Composite Design were established. They were modified to fit into calculation of non-linear constrained optimization problem. Optimization method was successfully applied to the calculation of the microparameters that gave fair match between the results from laboratory tests and those from uniaxial compression simulations.

Pore fluid solid particle coupling method was developed based on bonded particle model. Results obtained were in good agreement with what is known from corresponding experiments with geomaterials, especially the simulation of the biaxial compression test. Simulation results proved that presence of pore fluid and pore fluid pressure play a crucial role on the variation of strength and fracturing patterns in fluid saturated rocks. Modeling of coupled interaction between pore fluids and solid particles was developed and applied to biaxial compression simulations. Mechanical effect of pore fluid on strength and fracturing patterns were reproduced. Seismic characteristics of crack events were monitored and analyzed. Calculated b-values in dry, saturated rock models with pore fluid pressure exhibited similar tendency as observed in seismology. Dependency of b-values on pore fluid pressure was well captured. It is conclusive that the model prediction of mechanical and seismic behavior of rocks using the newly developed hydro-mechanical coupling captures most of the experimental observations, especially the effect of pore fluid pressure on rock strength and fracturing.

Mode II fracturing processes in dry and saturated rocks were investigated. Fracturing in mode II was technically induced by Punch Through Shear test. The results were compared with those obtained by simulations. It turned out that some of the results are consistent, for example, strength variation, formation of fracture process zone, etc. Hydro-mechanical coupling was applied to simulation of PTS test. It was observed that the peak strength decreased 20% due to the presence of pore fluid. Fluid concentration into the local cracks took part in further propagation and
branching of the local cracks. Coalescence of these local cracks led to clouds of crack clusters and formation of fracture process zone. In laboratory PTS experiments, the reduction of peak axial force and mode II fracture toughness due to saturation in granite were recorded 10~20%. Results were consistent with the estimation made earlier by simulation in which 10~20% of peak strength reduction was recorded under the presence of pore fluid of 0.1 MPa in pressure. At the point where brittle load drop stops in the axial load vs. axial displacement curve, different unloading stiffness in dry sample condition and saturated sample condition was recorded. It was found that the unloading stiffness in dry condition was little bit higher than that in saturated condition. The observed increase of stiffness in the post-peak regime is attributed to interlocking of the formed mode II fracture faces. Interlocking of the fractured surfaces was affected by the presence of pore fluid. Fluid concentration in the fracture reduces frictional resistance and hence enhances mobility of the fractured surfaces. Peak axial load variation in granite and sandstone under different loading rates were examined. A prominent difference in axial load versus axial displacement curves were noticed between granite and sandstone. In case of granite, there was not much difference in initial stiffness of the two curves, one for 0.2 mm/min and the other for 0.02 mm/min loading rate. However, in case of sandstone, stiffness reduced a lot. Interpretation on the test results is that when a saturated sample undergoes punch loading two zones are formed within the sample, one being compacted and the other being dilated. Pore fluid migration and local exchange occur between these two zones through the rock matrix. But in case of sandstone, pore fluid permeation takes less time to travel from the compacting zone through the rock matrix to reach the dilating zone due to low porosity rock matrix, hence it can easily degrade rock matrix’s strength. Fracture traces were inspected by impregnating the failed samples with epoxy resin and cut parallel to the fracture plane. Fractures in saturated granite samples exhibited sub-parallel fractures aligned in a wider zone compared to dry sample.

This study introduced a numerical method that can simulate the hydro-mechanical coupling. Laboratory experiments and numerical simulations were focused on the examination of confined shear fracturing and failure in saturated rocks, so that in situ settings of subsurface reservoir and underground caverns could be reflected as much as possible, where the nearby pre-existing fractures are likely exposed to confined shearing in saturated condition. The insights gained through this study may provide contributions to understanding shear-induced fracturing in combination with fluid, and how this interaction results in the degradation of material strength. Moreover, the correlation of the numerical simulations results to laboratory observations will allow for the improved assessment of hydro-mechanically coupled behavior of geo-materials.
SELECTED REFERENCES


Backers T. 2006. Personal communication.


